

Request Jan Delaval

Access DB# 127349

# SEARCH REQUEST FORM

Scientific and Technical Information Center

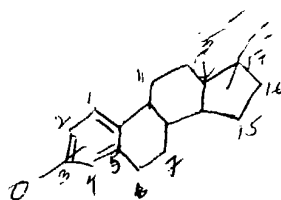
Requester's Full Name: Sabeha Qazi Examiner #: 74141 Date: 7/14/04  
Art Unit: 1616 Phone Number 301 20622 Serial Number 091893324  
Mail Box and Bldg/Room Location: 4C70 Results Format Preferred (circle) PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need. ME

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Alkyl ether modified Polycytosine  
Comps  
Inventors (please provide full names): Prokhor et al

Fig. 1 is a chemical structure of a polycytosine derivative, showing a polycyclic aromatic system with a cytosine base attached to a sugar moiety. The structure is labeled with various atoms and bonds, and includes a legend for the substituents R and X.



Please leave your

On

R can be alkyl.

st. chain, cyclic,  
unsaturated, saturated

Please see attached sheet

Thank you.

## STAFF USE ONLY

Type of Search: Jan Vendors and cost where applicable: 22504

Date Submitted: 7/20 Date Completed: 7/20  
Searcher Prep & Review Time: 15 Fulltext: Sequence Systems  
Clerical Prep Time: 40 Patent Family: WWW/Internet  
Online Time: 40 Other: Other (specify)

=> fil reg

FILE 'REGISTRY' ENTERED AT 11:27:37 ON 20 JUL 2004  
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Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 19 JUL 2004 HIGHEST RN 713066-32-1  
DICTIONARY FILE UPDATES: 19 JUL 2004 HIGHEST RN 713066-32-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

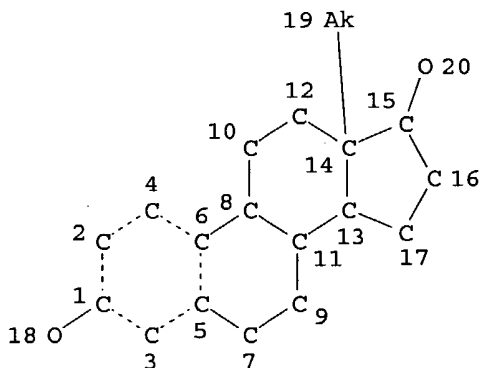
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d sta que l21

L9

STR



NODE ATTRIBUTES:

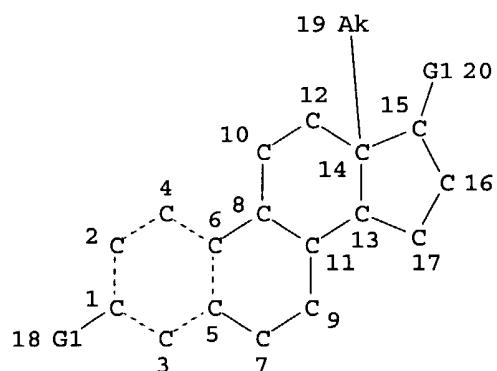
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CONNECT IS M1 RC AT 20  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 1  
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

L11 13381 SEA FILE=REGISTRY SSS FUL L9  
L12 STR



O—Ak  
@21 22

O—Cb  
@23 24

O—Ak—Cb  
@25 26 27

VAR G1=OH/21/23/25

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

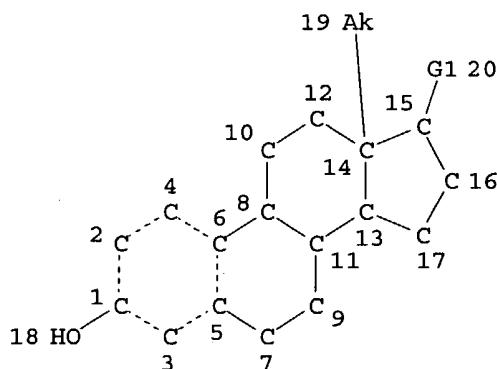
RSPEC 1

NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE

L14 434 SEA FILE=REGISTRY SUB=L11 CSS FUL L12

L19 STR



O—Ak  
@21 22

O—Cb  
@23 24

O—Ak—Cb  
@25 26 27

VAR G1=21/23/25

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 1

NUMBER OF NODES IS 27

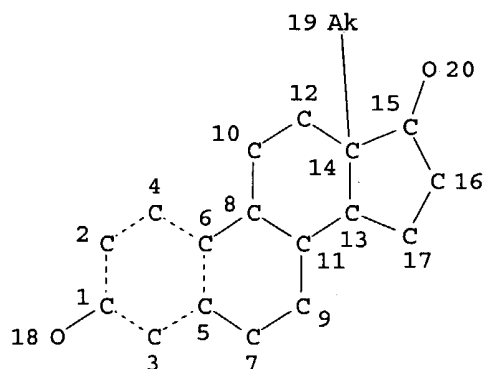
STEREO ATTRIBUTES: NONE

L20 23 SEA FILE=REGISTRY SUB=L14 SSS FUL L19

L21 22 SEA FILE=REGISTRY ABB=ON PLU=ON L20 NOT 13C#

=> => d sta que 125

L9 STR



## NODE ATTRIBUTES:

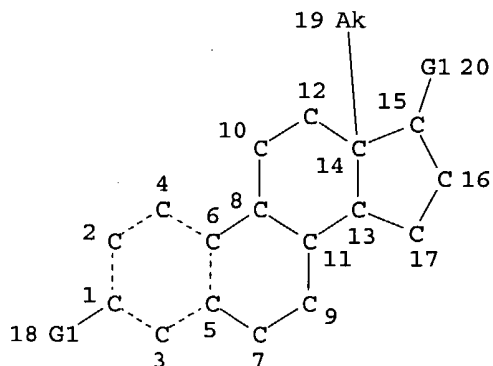
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 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RSPEC 1  
 NUMBER OF NODES IS 20

## STEREO ATTRIBUTES: NONE

L11 13381 SEA FILE=REGISTRY SSS FUL L9  
 L12 STR



O—Ak  
 @21 22

O—Cb  
 @23 24

O—Ak—Cb  
 @25 26 27

VAR G1=OH/21/23/25

## NODE ATTRIBUTES:

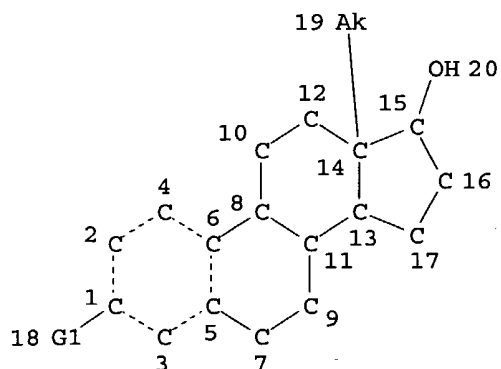
DEFAULT MLEVEL IS ATOM  
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## GRAPH ATTRIBUTES:

RSPEC 1  
 NUMBER OF NODES IS 27

## STEREO ATTRIBUTES: NONE

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 L15 119 SEA FILE=REGISTRY ABB=ON PLU=ON L14 AND NC>=2  
 L22 STR



O—Ak  
@21 22

O—Cb  
@23 24

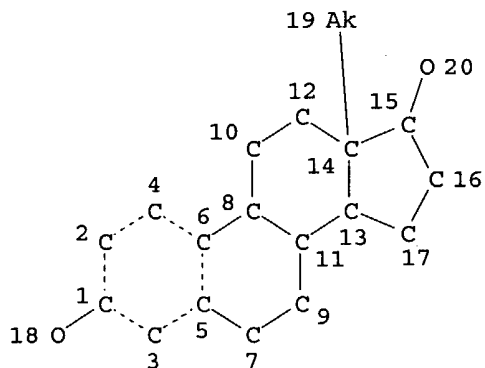
O—Ak—Cb  
@25 26 27

VAR G1=21/23/25  
NODE ATTRIBUTES:  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RSPEC 1  
NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE  
L23 99 SEA FILE=REGISTRY SUB=L14 SSS FUL L22  
L24 95 SEA FILE=REGISTRY ABB=ON PLU=ON L23 NOT L15  
L25 87 SEA FILE=REGISTRY ABB=ON PLU=ON L24 NOT (T OR D)/ELS

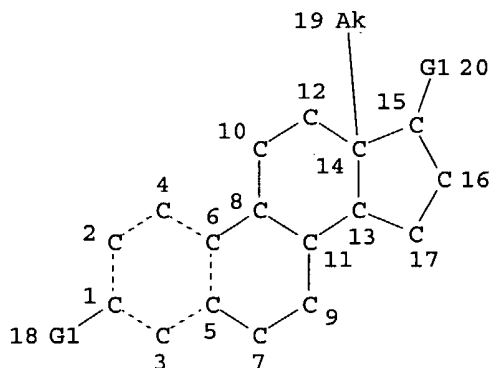
=> d sta que l32  
L9 STR



NODE ATTRIBUTES:  
CONNECT IS M1 RC AT 18  
CONNECT IS M1 RC AT 20  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RSPEC 1  
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE  
L11 13381 SEA FILE=REGISTRY SSS FUL L9  
L12 STR



O—Ak  
@21 22

$$\begin{array}{cc} \text{O} - \text{Cb} \\ @23 \quad 24 \end{array}$$

0—Ak—Cb  
@25 26 27

VAR G1=OH/21/23/25

**NODE ATTRIBUTES:**

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

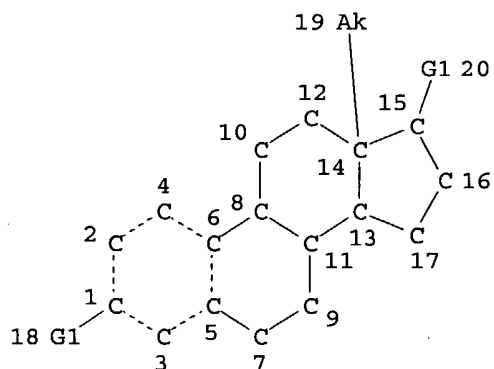
RSPEC 1

NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE

L14 434 SEA FILE=REGISTRY SUB=L11 CSS FUL L12

L30 STR



O—Ak  
@21 22

0—Cb  
@23 24

0—Ak—Cb  
@25 26 27

VAR G1=21/23/25

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 1

NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE

L31 58 SEA FILE=REGISTRY SUB=L14 SSS FUL L30

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L32      57 SEA FILE=REGISTRY ABB=ON  PLU=ON  L31 NOT (T OR D)/ELS
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=> d his

(FILE 'HOME' ENTERED AT 10:33:36 ON 20 JUL 2004)  
SET COST OFF

FILE 'HCAPLUS' ENTERED AT 10:34:03 ON 20 JUL 2004

L1 1 S US20020035100/PN OR (US2001-893324# OR WO2001-US41170 OR US20  
E PROKAI L/AU  
L2 122 S E3,E4,E7  
E SIMPKINS J/AU  
L3 245 S E3,E5,E7-E9  
SEL RN L1

FILE 'REGISTRY' ENTERED AT 10:35:20 ON 20 JUL 2004

L4 18 S E1-E18  
L5 16 S L4 AND C5-C6-C6-C6/ES  
L6 9 S L5 AND 4/NR  
L7 7 S L5 NOT L6  
L8 STR  
L9 STR L8  
L10 50 S L9  
L11 13381 S L9 FUL  
SAV TEMP L11 QAZI893/A  
L12 STR L9  
L13 22 S L12 CSS SAM SUB=L11  
L14 434 S L12 CSS FUL SUB=L11  
SAV L14 QAZI893A/A  
L15 119 S L14 AND NC>=2  
L16 13 S L15 NOT ((MXS OR PMS OR IDS)/CI OR COMPD OR WITH OR UNSPECIFI  
L17 2 S L16 NOT C18H24O2  
L18 11 S L16 NOT L17  
L19 STR L12  
L20 23 S L19 FUL SUB=L14  
SAV L20 QAZI893B/A  
L21 22 S L20 NOT 13C#  
L22 STR L19  
L23 99 S L22 FUL SUB=L14  
SAV L23 QAZI893C/A  
L24 95 S L23 NOT L15  
L25 87 S L24 NOT (T OR D)/ELS  
L26 12 S L23 NOT L25  
L27 9 S L26 AND C19H26O2  
L28 3 S L26 AND C19H26O2 NOT (T OR D)/ELS  
L29 2 S L28 NOT CYCLODEXTRIN  
L30 STR L19  
L31 58 S L30 FUL SUB=L14  
SAV L31 QAZI893D/A  
L32 57 S L31 NOT (T OR D)/ELS  
L33 169 S L5,L17,L21,L25,L29,L32  
SAV L33 QAZI893E/A  
L34 168 S L33 NOT (T OR D)/ELS  
L35 149 S L14 NOT L15,L34  
L36 89 S L35 NOT (T OR D)/ELS  
L37 46 S L36 NOT IDS/CI  
L38 41 S L37 NOT (11C# OR 13C# OR 14C#)  
L39 39 S L38 NOT PMS/CI

FILE 'HCAPLUS' ENTERED AT 11:19:38 ON 20 JUL 2004

L40 52840 S L34  
L41 1346 S L39  
L42 53115 S L40,L41  
L43 98 S L1-L3 AND L42

FILE 'REGISTRY' ENTERED AT 11:20:19 ON 20 JUL 2004

L44 1 S 50-28-2  
L45 167 S L34 NOT L44  
L46 38 S L39 NOT 57-91-0

FILE 'HCAPLUS' ENTERED AT 11:21:54 ON 20 JUL 2004

L47 605 S L45  
L48 148 S L46  
L49 715 S L47,L48  
L50 9 S L1-L3 AND L49  
L51 706 S L49 NOT L50  
L52 654 S L51 AND (PD<=20000627 OR AD<=20000627 OR PRD<=20000627)

FILE 'REGISTRY' ENTERED AT 11:24:14 ON 20 JUL 2004

L53 33 S L45,L46 AND (C26H40O2 OR C24H36O2 OR C22H32O2)  
L54 5 S L20 AND L53  
L55 28 S L53 NOT L54  
L56 18 S L20 NOT L54  
L57 17 S L56 NOT L3C#

FILE 'HCAPLUS' ENTERED AT 11:26:54 ON 20 JUL 2004

L58 41 S L54 OR L57  
L59 33 S L58 AND L52

FILE 'USPATFULL, USPAT2' ENTERED AT 11:27:18 ON 20 JUL 2004

L60 5 S L54 OR L57

FILE 'REGISTRY' ENTERED AT 11:27:37 ON 20 JUL 2004

=> fil uspatall

FILE 'USPATFULL' ENTERED AT 11:29:09 ON 20 JUL 2004

CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPAT2' ENTERED AT 11:29:09 ON 20 JUL 2004

CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

=> d l60 bib abs hitstr tot

L60 ANSWER 1 OF 5 USPATFULL on STN

AN 2002:340319 USPATFULL

TI Extended release growth promoting two component composition

IN Cady, Susan Mancini, Yardley, PA, United States

Macar, Claude, Paris, FRANCE

Gibson, John W., Springville, AL, United States

PA Akzo Nobel N.V., Amhem, NETHERLANDS (non-U.S. corporation)

Southern BioSystems, Birmingham, AL, United States (U.S. corporation)

PI US 6498153 B1 20021224

AI US 1999-273862 19990322 (9)

PRAI FR 1998-16707 19981231

DT Utility

FS GRANTED

EXNAM Primary Examiner: Badio, Barbara P.

LREP Blackstone, William M.

CLMN Number of Claims: 46

ECL Exemplary Claim: 1

DRWN 0 Drawing Figure(s); 0 Drawing Page(s)

LN.CNT 776

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB An extended release composition comprising a first composition comprising growth promoters and a second composition comprising growth promoters and a biodegradable polymer is described. A method of increasing weight gain in food animals utilizing the composition, a pharmaceutical dosage form containing the composition and a method of preparing the pharmaceutical dosage form are also described, as are pellets of the composition for implantation in food animals.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 55561-42-7

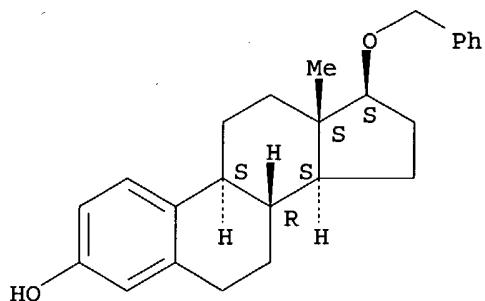
(pellets containing growth promoters and biodegradable polymers for

controlled-release implants for farm animals)

RN 55561-42-7 USPATFULL

CN Estra-1,3,5(10)-trien-3-ol, 17-(phenylmethoxy)-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L60 ANSWER 2 OF 5 USPATFULL on STN

AN 2002:61264 USPATFULL

TI Alkyl ether modified polycyclic compounds having a terminal phenol and uses for protection of cells

IN Prokai, Laszlo, Gainesville, FL, UNITED STATES  
Simpkins, James W., Fort Worth, TX, UNITED STATES

PI US 2002035100 A1 20020321

AI US 2001-893324 A1 20010627 (9)

PRAI US 2000-214077P 20000627 (60)

DT Utility

FS APPLICATION

LREP BROMBERG & SUNSTEIN LLP, 125 SUMMER STREET, BOSTON, MA, 02110-1618

CLMN Number of Claims: 46

ECL Exemplary Claim: 1

DRWN 5 Drawing Page(s)

LN.CNT 951

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Methods and compositions are provided for achieving a cytoprotective effect by selecting a polycyclic compound with a phenol group at one end of the molecule and a carbon ring at the other such that an alkyl ether functional group in which the alkyl group has a formula  $C_{nH_{2n+1}}$  (where n is at least 3 and less than 20) is positioned on the carbon ring. The compound may be used to achieve a cytoprotective effect in cells and to retard the development of a degenerative condition in a subject suffering from a disease, trauma or aging.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

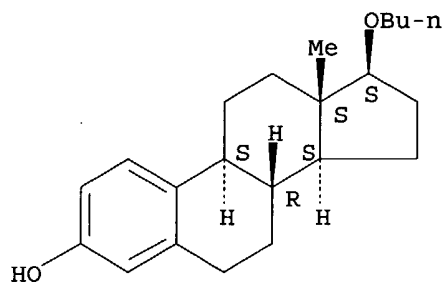
IT 319427-05-9P

(crystal structure)

RN 319427-05-9 USPATFULL

CN Estra-1,3,5(10)-trien-3-ol, 17-butoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 4954-12-5P 319427-03-7P 319427-04-8P

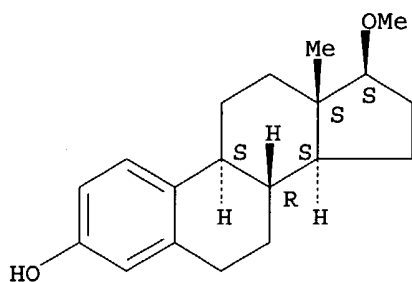
319427-06-0P 319427-07-1P

(preparation of 17β- or 3-alkyl ether derivs. of estradiol used for  
cytoprotective activity of cells from degeneration)

RN 4954-12-5 USPATFULL

CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX  
NAME)

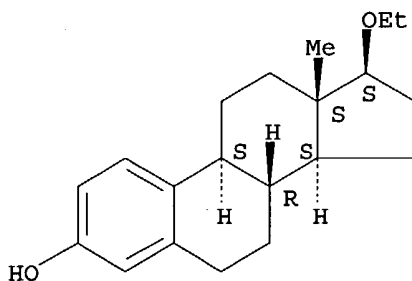
Absolute stereochemistry.



RN 319427-03-7 USPATFULL

CN Estra-1,3,5(10)-trien-3-ol, 17-ethoxy-, (17β)- (9CI) (CA INDEX NAME)

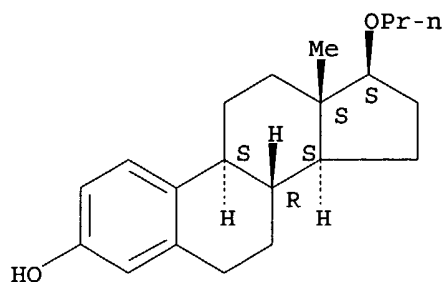
Absolute stereochemistry.



RN 319427-04-8 USPATFULL

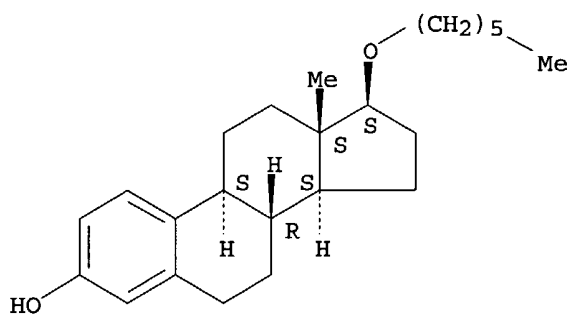
CN Estra-1,3,5(10)-trien-3-ol, 17-propoxy-, (17β)- (9CI) (CA INDEX  
NAME)

Absolute stereochemistry.



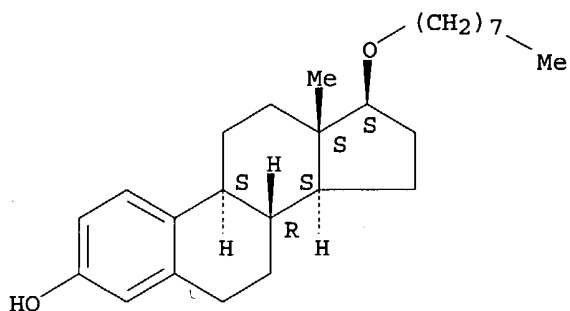
RN 319427-06-0 USPATFULL  
 CN Estra-1,3,5(10)-trien-3-ol, 17-(hexyloxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 319427-07-1 USPATFULL  
 CN Estra-1,3,5(10)-trien-3-ol, 17-(octyloxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L60 ANSWER 3 OF 5 USPATFULL on STN  
 AN 1999:7375 USPATFULL  
 TI Steroid inhibitors of estrone sulfatase and associated pharmaceutical compositions and methods of use  
 IN Tanabe, Masato, Palo Alto, CA, United States  
 Peters, Richard H., San Jose, CA, United States  
 Chao, Wan-Ru, Sunnyvale, CA, United States  
 Shigeno, Kazuhiko, Mountain View, CA, United States  
 PA SRI International, Menlo Park, CA, United States (U.S. corporation)  
 PI US 5861388 19990119  
 AI US 1997-1601 19971231

RLI Division of Ser. No. US 1997-794229, filed on 29 Jan 1997, now patented,  
 Pat. No. US 5763432  
 DT Utility  
 FS Granted  
 EXNAM Primary Examiner: Dees, Jose G.; Assistant Examiner: Bodio, Barbara  
 LREP Reed, Dianne E.Bozicevic & Reed LLP  
 CLMN Number of Claims: 22  
 ECL Exemplary Claim: 1  
 DRWN No Drawings  
 LN.CNT 1778

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Novel compounds useful as inhibitors of estrone sulfatase are provided.  
 The compounds have the structural formula (I) ##STR1## wherein X and Y,  
 or Y and Z, form an oxathiazine dioxide ring or a dihydro-oxathiazine  
 dioxide ring, and the other various substituents are as defined herein.  
 Pharmaceutical compositions and methods for using the compounds of  
 formula (I) to treat estrogen-dependent disorders are provided as well.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

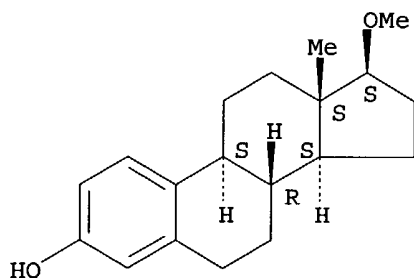
IT 4954-12-5

(preparation of steroid inhibitors of estrone sulfatase)

RN 4954-12-5 USPATFULL

CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX  
 NAME)

Absolute stereochemistry.



L60 ANSWER 4 OF 5 USPATFULL on STN

AN 1998:65215 USPATFULL

TI Steroid inhibitors of estrone sulfatase and associated pharmaceutical  
 compositions and methods of use

IN Tanabe, Masato, Palo Alto, CA, United States

Peters, Richard H., San Jose, CA, United States

Chao, Wan-Ru, Sunnyvale, CA, United States

Shigeno, Kazuhiko, Mountain View, CA, United States

PA SRI International, Menlo Park, CA, United States (U.S. corporation)

PI US 5763432 19980609

AI US 1997-794229 19970129 (8)

DT Utility

FS Granted

EXNAM Primary Examiner: Dees, Jose G.; Assistant Examiner: Badio, Barbara

LREP Reed, Dianne E.Bozicevic & Reed LLP

CLMN Number of Claims: 13

ECL Exemplary Claim: 1

DRWN No Drawings

LN.CNT 1700

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Novel compounds useful as inhibitors of estrone sulfatase are provided.  
 The compounds have the structural formula (I) ##STR1## wherein X and Y,  
 or Y and Z, form an oxathiazine dioxide ring or a dihydro-oxathiazine

dioxide ring, and the other various substituents are as defined herein. Pharmaceutical compositions and methods for using the compounds of formula (I) to treat estrogen-dependent disorders are provided as well.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

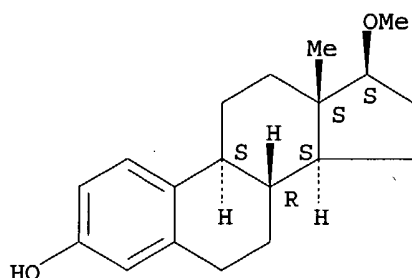
IT 4954-12-5

(preparation of steroid inhibitors of estrone sulfatase)

RN 4954-12-5 USPATFULL

CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L60 ANSWER 5 OF 5 USPATFULL on STN

AN 96:82674 USPATFULL

TI Methods for neuroprotection

IN Simpkins, James W., Gainesville, FL, United States

Singh, Meharvan, Gainesville, FL, United States

Bishop, Jean, Jacksonville, FL, United States

PA University of Florida, Gainesville, FL, United States (U.S. corporation)

PI US 5554601 19960910

AI US 1994-318042 19941004 (8)

RLI Continuation-in-part of Ser. No. US 1993-149175, filed on 5 Nov 1993, now abandoned

DT Utility

FS Granted

EXNAM Primary Examiner: Weddington, Kevin E.

LREP Bromberg & Sunstein

CLMN Number of Claims: 29

ECL Exemplary Claim: 1

DRWN 11 Drawing Figure(s); 10 Drawing Page(s)

LN.CNT 1532

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB A method is provided for conferring neuroprotection on a population of cells using estrogen compounds that have insubstantial sex activity and furthermore, a method is provided that utilizes estrogen compounds in the absence of testosterone for treating neurodegenerative diseases including Alzheimer's disease so as to retard the adverse effects of these disorders, Examples of estrogen compounds that have insubstantial sex activity includes alpha isomers of estrogen compounds such as 17 $\alpha$  estradiol.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

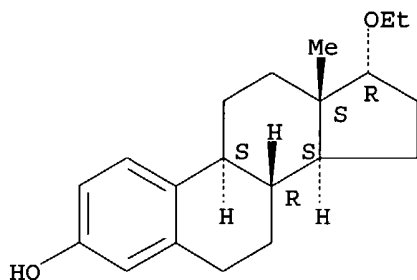
IT 182624-49-3 182624-51-7 182823-27-4

(methods for neuroprotection)

RN 182624-49-3 USPATFULL

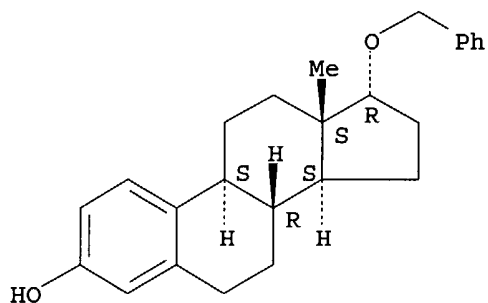
CN Estra-1,3,5(10)-trien-3-ol, 17-ethoxy-, (17 $\alpha$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



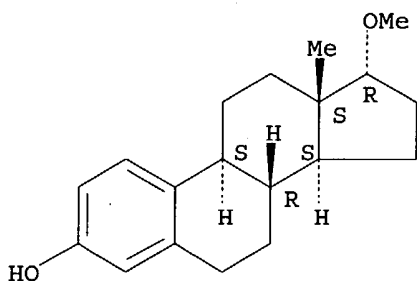
RN 182624-51-7 USPATFULL  
 CN Estra-1,3,5(10)-trien-3-ol, 17-(phenylmethoxy)-, (17α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 182823-27-4 USPATFULL  
 CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 11:29:20 ON 20 JUL 2004

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FILE COVERS 1907 - 20 Jul 2004 VOL 141 ISS 4  
FILE LAST UPDATED: 19 Jul 2004 (20040719/ED)

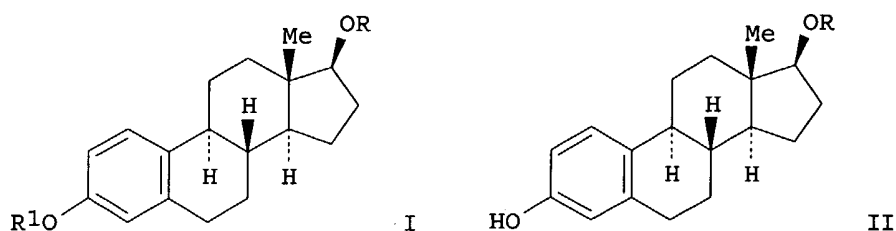
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d all hitstr tot 150

L50 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN  
AN 2002:10439 HCAPLUS  
DN 136:85991  
ED Entered STN: 04 Jan 2002  
TI Preparation of 17 $\beta$ -alkyl ether estradiol derivatives with  
cytoprotective activity of cells from degeneration through disease, trauma  
or aging  
IN Prokai, Laszlo; Simpkins, James W.  
PA University of Florida Research Foundation, Inc., USA  
SO PCT Int. Appl., 29 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
IC ICM C07D  
CC 32-3 (Steroids)  
Section cross-reference(s): 1, 75  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002000619	A2	20020103	WO 2001-US41170	20010627 <--
	WO 2002000619	A3	20020829		
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	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
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	US 2002035100	A1	20020321	US 2001-893324	20010627 <--
	EP 1294446	A2	20030326	EP 2001-955052	20010627 <--
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
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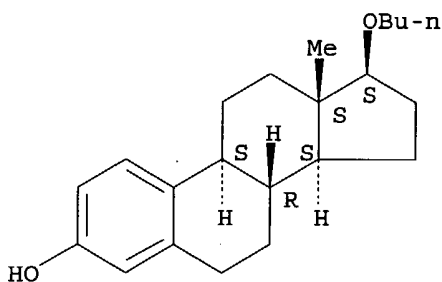
GI



- AB    Cytoprotective compds. I (R = Me, Et, Pr, Bu, (CH<sub>2</sub>)<sub>5</sub>Me, or (CH<sub>2</sub>)<sub>7</sub>Me; R<sub>1</sub> = OH) were prepared in 50-75% yields from 17 $\beta$ -estradiol. 17 $\beta$ -Estradiol and benzyl halide in K<sub>2</sub>CO<sub>3</sub> gave 93% yield of 3-benzyloxyestra-1,3,5(10)-trien-17 $\beta$ -ol which was then alkylated with the appropriate alkyl halides in DMF and NaH yielding the 3-benzyloxy protected derivs. of I which were then deprotected via catalytic hydrogenation using ammonium formate in Pd/C. Thus compds. II (R = hexyl and octyl) were prepared in 70 and 75% resp., and were neuroprotective to a similar extent at a concentration of 10  $\mu$ M and 1  $\mu$ M. Typical compns. contain approx. 0.01-95% by weight of active ingredient and the percentage of active ingredient will depend upon the dosage form and mode of administration; an ED of the active agent as measured in the plasma of a subject may be in the range of 5pg/mL-5000pg/mL. Cytoprotective compds. I (R = OH; R<sub>1</sub> = Bu, (CH<sub>2</sub>)<sub>7</sub>Me) were prepared from 17 $\beta$ -estradiol and Bu or octyl bromide in K<sub>2</sub>CO<sub>3</sub> in 68 and 72% resp.
- ST    estradiol hydroxy alkylated deriv prepn cytoprotective compn; neuroprotective alkyl ether steroid prepn; crystal structure butoxyestratrienol
- IT    Steroids, preparation  
 RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (alkylation of 17 $\beta$ -OH or 3-OH; preparation of 17 $\beta$ - or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)
- IT    Cytoprotective agents  
 (cardioprotective; preparation of 17 $\beta$ - or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)
- IT    Nervous system, disease  
 (degeneration; preparation of 17 $\beta$ - or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)
- IT    Alkylation  
 (hydroxyalkylation; preparation of 17 $\beta$ - or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)
- IT    Eye, disease  
 (macula, degeneration; preparation of 17 $\beta$ - or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)
- IT    Crystal structure  
 (of 17 $\beta$ -butoxyestra-1,3,5(10)-trien-3-ol)
- IT    Estrogen receptors  
 RL: BSU (Biological study, unclassified); BIOL (Biological study)  
 (preparation of 17 $\beta$ - or 3-alkyl ether derivs. of estradiol used as cytoprotective agents of cells from degeneration)
- IT    Anti-Alzheimer's agents  
 Anti-ischemic agents  
 Bone, disease  
 Drug delivery systems  
 (preparation of 17 $\beta$ - or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)
- IT    Osteoporosis  
 (therapeutic agents; preparation of 17 $\beta$ - or 3-alkyl ether derivs. of

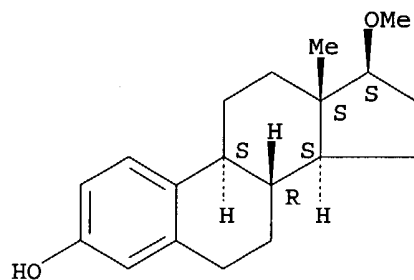
- estradiol used for cytoprotective activity of cells from degeneration)
- IT 319427-05-9P  
 RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (crystal structure)
- IT 4954-12-5P 21830-24-0P 128805-68-5P  
 319427-03-7P 319427-04-8P 319427-06-0P  
 319427-07-1P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of 17 $\beta$ - or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)
- IT 50-28-2, 17 $\beta$ -Estradiol, reactions 109-65-9, Butyl bromide  
 111-83-1, Octyl bromide  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of 17 $\beta$ - or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)
- IT 14982-15-1P 141318-37-8P 319426-98-7P  
 319426-99-8P 319427-00-4P 319427-01-5P  
 319427-02-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of 17 $\beta$ - or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)
- IT 319427-05-9P  
 RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (crystal structure)
- RN 319427-05-9 HCAPLUS  
 CN Estra-1,3,5(10)-trien-3-ol, 17-butoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



- IT 4954-12-5P 21830-24-0P 128805-68-5P  
 319427-03-7P 319427-04-8P 319427-06-0P  
 319427-07-1P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of 17 $\beta$ - or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)
- RN 4954-12-5 HCAPLUS  
 CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

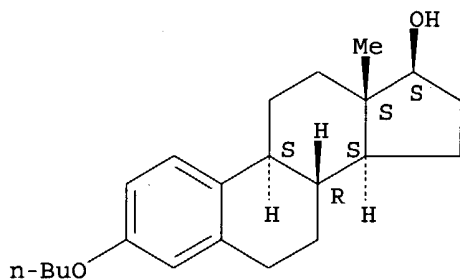
Absolute stereochemistry.



RN 21830-24-0 HCAPLUS

CN Estra-1,3,5(10)-trien-17-ol, 3-butoxy-, (17β)- (9CI) (CA INDEX NAME)

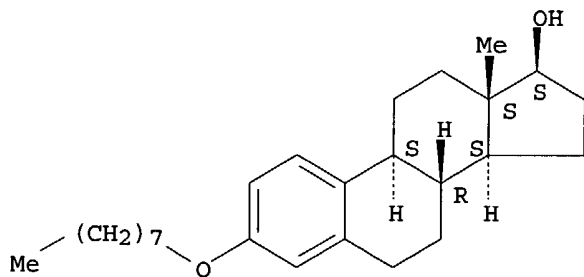
Absolute stereochemistry.



RN 128805-68-5 HCAPLUS

CN Estra-1,3,5(10)-trien-17-ol, 3-(octyloxy)-, (17β)- (9CI) (CA INDEX NAME)

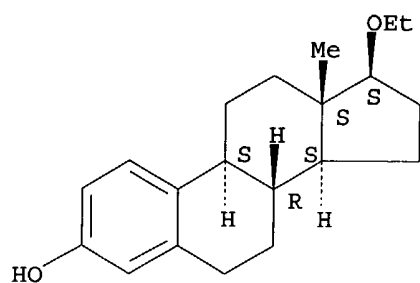
Absolute stereochemistry.



RN 319427-03-7 HCAPLUS

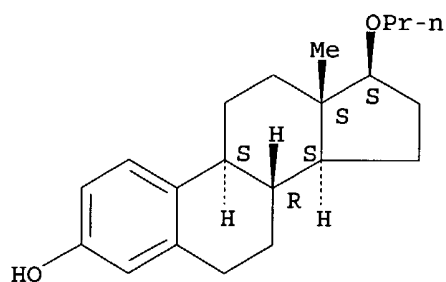
CN Estra-1,3,5(10)-trien-3-ol, 17-ethoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



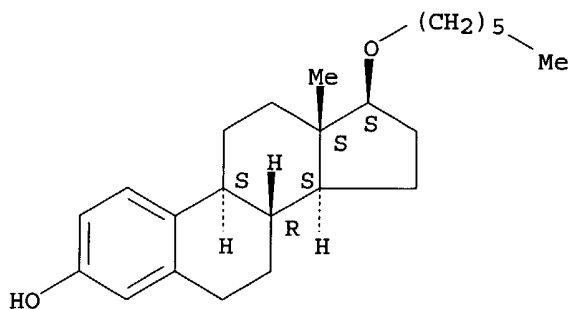
RN 319427-04-8 HCAPLUS  
 CN Estra-1,3,5(10)-trien-3-ol, 17-propoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



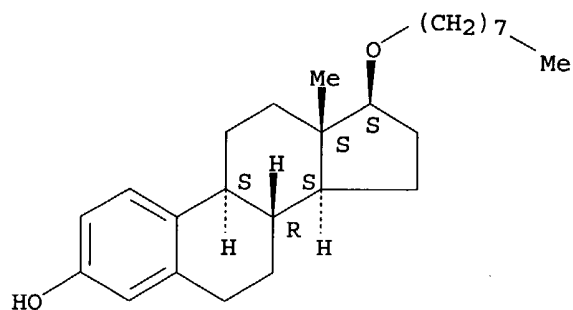
RN 319427-06-0 HCAPLUS  
 CN Estra-1,3,5(10)-trien-3-ol, 17-(hexyloxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 319427-07-1 HCAPLUS  
 CN Estra-1,3,5(10)-trien-3-ol, 17-(octyloxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 14982-15-1P 141318-37-8P 319426-98-7P  
 319426-99-8P 319427-00-4P 319427-01-5P  
 319427-02-6P

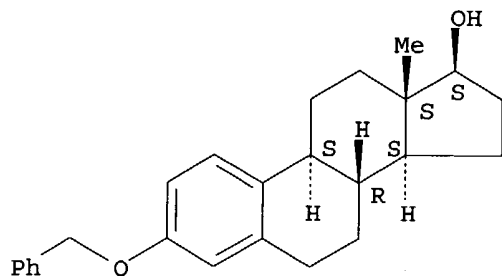
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)

(preparation of 17β- or 3-alkyl ether derivs. of estradiol used for  
 cytoprotective activity of cells from degeneration)

RN 14982-15-1 HCAPLUS

CN Estra-1,3,5(10)-trien-17-ol, 3-(phenylmethoxy)-, (17β)- (9CI) (CA  
 INDEX NAME)

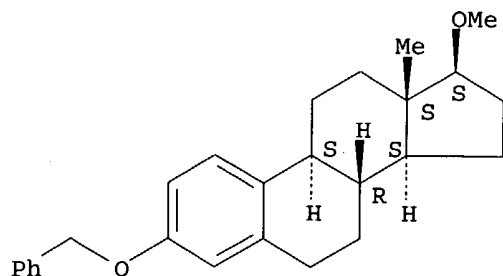
Absolute stereochemistry.



RN 141318-37-8 HCAPLUS

CN Estra-1,3,5(10)-triene, 17-methoxy-3-(phenylmethoxy)-, (17β)- (9CI)  
 (CA INDEX NAME)

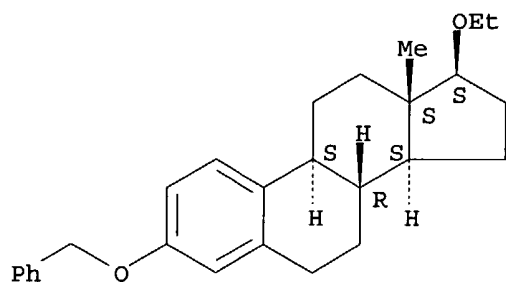
Absolute stereochemistry.



RN 319426-98-7 HCAPLUS

CN Estra-1,3,5(10)-triene, 17-ethoxy-3-(phenylmethoxy)-, (17β)- (9CI)  
 (CA INDEX NAME)

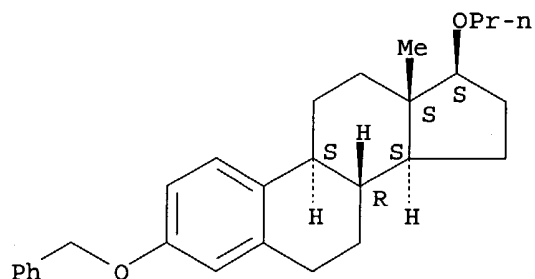
Absolute stereochemistry.



RN 319426-99-8 HCAPLUS

CN Estra-1,3,5(10)-triene, 3-(phenylmethoxy)-17-propoxy-, (17β)- (9CI)  
(CA INDEX NAME)

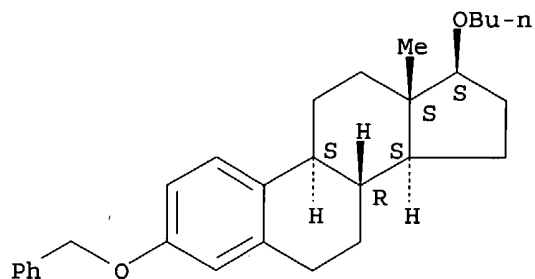
Absolute stereochemistry.



RN 319427-00-4 HCAPLUS

CN Estra-1,3,5(10)-triene, 17-butoxy-3-(phenylmethoxy)-, (17β)- (9CI)  
(CA INDEX NAME)

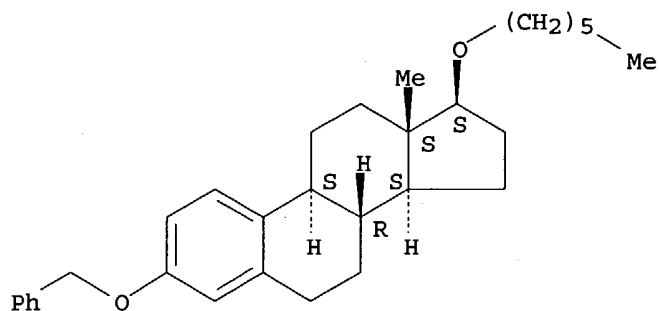
Absolute stereochemistry.



RN 319427-01-5 HCAPLUS

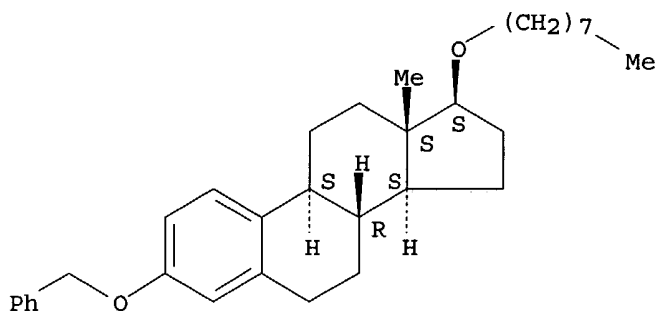
CN Estra-1,3,5(10)-triene, 17-(hexyloxy)-3-(phenylmethoxy)-, (17β)-  
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 319427-02-6 HCAPLUS  
 CN Estra-1,3,5(10)-triene, 17-(octyloxy)-3-(phenylmethoxy)-, (17β)-  
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L50 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2001:428147 HCAPLUS  
 DN 135:221441  
 ED Entered STN: 13 Jun 2001  
 TI Membrane fluidity effects of estratrienes  
 AU Liang, Y.; Belford, S.; Tang, F.; Prokai, L.; Simpkins, J.  
 W.; Hughes, J. A.  
 CS Department of Pharmaceutics, University of Florida, Gainesville, FL, USA  
 SO Brain Research Bulletin (2001), 54(6), 661-668  
 CODEN: BRBUDU; ISSN: 0361-9230  
 PB Elsevier Science Inc.  
 DT Journal  
 LA English  
 CC 2-4 (Mammalian Hormones)  
 AB Estrogens have demonstrable neuroprotective effects. This fact has lead to the proposed use of estrogens for the prevention and/or treatment of Alzheimer's disease. The exact protective mechanism estrogens provide is not fully understood. In this report, a potential non-genomic mechanism for estratrienes involving alterations in membrane fluidity was studied. Steroids, such as estrogen, are known to be membrane-active and can alter the lipid packing. In this study the authors used fluorescent methodologies to address the effect of naturally occurring steroids (17α- and 17β-estradiol, testosterone, and progesterone) and new estratriene analogs on membrane fluidity using liposomes and HT-22 hippocampal cells. The study's results indicate steroids, based on the estratriene nucleus, can modulate lipid packing as evidenced by (1) decreased membrane fusion events and (2) decreased membrane fluidity. The effects on the membrane were both time- and concentration-dependent. It was also

demonstrated through rational design estratriene analogs can be synthesized with enhanced membrane effects. Finally, in a glutamate-induced toxicity HT-22 model, the authors also demonstrated cellular protection with the estratriene-based mols. and analogs. The data suggest the plethora of cellular actions of estrogens may relate to or be influenced by membrane effects of the steroid.

- ST cell membrane fluidity estratriene; estradiol membrane fluidity  
 IT Animal cell line  
     (HT-22; estratrienes effects on membrane fluidity)  
 IT Membrane, biological  
     (bilayer; estratrienes effects on membrane fluidity)  
 IT Liposomes  
     (estratrienes effects on membrane fluidity)  
 IT Phosphatidylethanolamines, biological studies  
   Phosphatidylserines  
   RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL  
     (Biological study); PROC (Process)  
     (estratrienes effects on membrane fluidity)  
 IT Brain  
     (hippocampus; estratrienes effects on membrane fluidity)  
 IT 57-88-5, Cholesterol, biological studies  
   RL: BAC (Biological activity or effector, except adverse); BPR (Biological  
     process); BSU (Biological study, unclassified); BIOL (Biological study);  
     PROC (Process)  
     (estratrienes effects on membrane fluidity)  
 IT 50-28-2, 17 $\beta$ -Estradiol, biological studies 53-63-4,  
   Estra-1,3,5(10)-trien-3-ol 57-83-0, Progesterone, biological studies  
   57-91-0, 17 $\alpha$ -Estradiol 58-22-0, Testosterone  
   RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
     study, unclassified); BIOL (Biological study)  
     (estratrienes effects on membrane fluidity)  
 IT **319427-07-1P**  
   RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
     study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL  
     (Biological study); PREP (Preparation)  
     (estratrienes effects on membrane fluidity)  
 IT 50-50-0, 17 $\beta$ -Estradiol 3-benzoate  
   RL: RCT (Reactant); RACT (Reactant or reagent)  
     (estratrienes effects on membrane fluidity)

RE.CNT 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD  
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IT 319427-07-1P

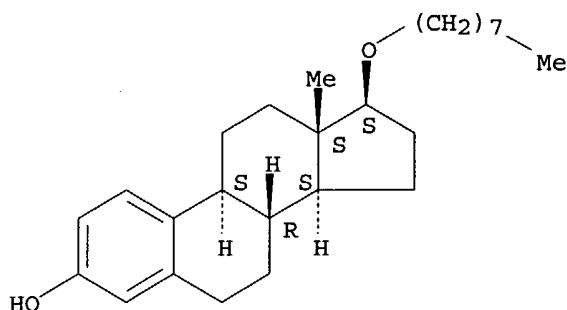
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(estratrienes effects on membrane fluidity)

RN 319427-07-1 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-(octyloxy)-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L50 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2001:114973 HCAPLUS

DN 134:158108

ED Entered STN: 15 Feb 2001

TI Methods of cytoprotection using an enantiomer of estrogen of ischemic damage

IN Covey, Douglas F.; Simpkins, James W.

PA University of Florida Research Foundation, Inc., USA; Apollo Biopharmaceutics Inc.; Washington University

SO PCT Int. Appl., 58 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM A61K031-00

CC 2-4 (Mammalian Hormones)

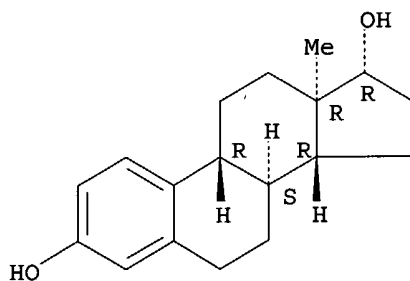
## Section cross-reference(s): 32

FAN.CNT 9

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PI	WO 2001010430	A2	20010215	WO 2000-US22163	20000811
	WO 2001010430	A3	20010830		
	WO 2001010430	C2	20020711		
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	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	US 6350739	B1	20020226	US 1999-372627	19990811
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	EP 1143947	A3	20020911		
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	JP 2003510336	T2	20030318	JP 2001-526632	20000811
PRAI	US 1999-372627	A	19990811		
	WO 2000-US22163	W	20000811		
AB	The present invention in various embodiments provides methods of cytoprotection and treatment of disease that include providing an enantiomer of an estrogen compound to a population of cells in a subject with a cytodegenerative condition to protect those cells from further damage. The enantiomer of the invention is specifically, ent-17 $\beta$ -estradiol or ent-17 $\beta$ -estradiol 17-acetate. Examples of cytodegenerative conditions include stroke and neurodegenerative diseases. The invention further discloses a method of synthesis of ent-17 $\beta$ -estradiol and ent-17 $\beta$ -estradiol 17-acetate. A pharmaceutical formulation comprising an estrogen enantiomer in an oil is also claimed.				
ST	estrogen enantiomer prepn cytoprotection				
IT	Cytoprotective agents (cardioprotective; methods of cytoprotection using synthetically prepared estrogen enantiomers)				
IT	Brain, disease (cerebrovascular, ischemic event; methods of cytoprotection using synthetically prepared estrogen enantiomers)				
IT	Nervous system (degeneration, treatment; methods of cytoprotection using synthetically prepared estrogen enantiomers)				
IT	Estrogens RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (enantiomers; methods of cytoprotection using synthetically prepared estrogen enantiomers)				
IT	Cytoprotective agents (endothelial protection; methods of cytoprotection using synthetically prepared estrogen enantiomers)				
IT	Heart, disease (infarction, ischemic event; methods of cytoprotection using synthetically prepared estrogen enantiomers)				
IT	Surgery (ischemic event; methods of cytoprotection using synthetically prepared estrogen enantiomers)				
IT	Anti-Alzheimer's agents Anti-ischemic agents Cytoprotective agents (methods of cytoprotection using synthetically prepared estrogen enantiomers)				
IT	Cytoprotective agents (neuroprotectants; methods of cytoprotection using synthetically prepared estrogen enantiomers)				

- IT Drug delivery systems  
(oily; methods of cytoprotection using oily pharmaceutical formulations containing estrogen enantiomers)
- IT Bone, disease  
(osteodegenerative disease treatment; methods of cytoprotection using synthetically prepared estrogen enantiomers)
- IT Brain, disease  
(stroke, ischemic event; methods of cytoprotection using synthetically prepared estrogen enantiomers)
- IT Meninges  
(subarachnoid hemorrhage, ischemic event; methods of cytoprotection using synthetically prepared estrogen enantiomers)
- IT Injury  
(trauma, ischemic event; methods of cytoprotection using synthetically prepared estrogen enantiomers)
- IT Osteoporosis  
(treatment; methods of cytoprotection using synthetically prepared estrogen enantiomers)
- IT 300853-33-2P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(methods of cytoprotection using synthetically prepared estrogen enantiomers)
- IT 3736-22-9P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(methods of cytoprotection using synthetically prepared estrogen enantiomers)
- IT 139973-49-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(methods of cytoprotection using synthetically prepared estrogen enantiomers)
- IT 4091-86-5P 185685-33-0P 325808-57-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(methods of cytoprotection using synthetically prepared estrogen enantiomers)
- IT 3736-22-9P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(methods of cytoprotection using synthetically prepared estrogen enantiomers)
- RN 3736-22-9 HCAPLUS
- CN Estra-1,3,5(10)-triene-3,17-diol, (8 $\alpha$ ,9 $\beta$ ,13 $\alpha$ ,14 $\beta$ ,17.  
alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L50 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN  
AN 2001:51133 HCAPLUS  
DN 134:126193  
ED Entered STN: 21 Jan 2001  
TI The nonfeminizing enantiomer of 17 $\beta$ -estradiol exerts protective effects in neuronal cultures and a rat model of cerebral ischemia  
AU Green, P. S.; Yang, S.-H.; Nilsson, K. R.; Kumar, A. S.; Covey, D. F.; Simpkins, J. W.  
CS Center for the Neurobiology of Aging, University of Florida, Gainesville, FL, 32610, USA  
SO Endocrinology (2001), 142(1), 400-406  
CODEN: ENDOAO; ISSN: 0013-7227  
PB Endocrine Society  
DT Journal  
LA English  
CC 2-4 (Mammalian Hormones)  
AB Estrogens are potent neuroprotective compds. in a variety of animal and cell culture models, and data indicate that estrogen receptor (ER)-mediated gene transcription is not required for some of these effects. To further address the requirement for an ER in estrogen enhancement of neuronal survival, the authors assessed the enantiomer of 17 $\beta$ -estradiol (Ent-E2), which has identical chemical properties but interacts only weakly with known ERs, for neuroprotective efficacy. Ent-E2 was both as potent and efficacious as 17 $\beta$ -estradiol in attenuating oxidative stress-induced death in HT-22 cells, a murine hippocampal cell line. Further, Ent-E2 completely attenuated H2O2 toxicity in human SK-N-SH neuroblastoma cells at a 10 nM concentration. In a rodent model of focal ischemia, 17 $\beta$ -estradiol (100  $\mu$ g/kg) or Ent-E2 (100  $\mu$ g/kg), injected 2 h before middle cerebral artery occlusion, resulted in a 60 and 61% reduction in lesion volume, resp. Ent-E2, at the doses effective in this study, did not stimulate uterine growth or vaginal opening in juvenile female rats when administered daily for 3 days. These data indicate that the neuroprotective effects of estrogens, both in vitro and in vivo, can be disassocd. from the peripheral estrogenic actions.  
ST estradiol enantiomer neuroprotectant cerebral ischemia  
IT Brain  
(hippocampus; nonfeminizing enantiomer of 17 $\beta$ -estradiol exerts protective effects in neuronal cultures and rat model of cerebral ischemia)  
IT Brain, disease  
(ischemia, focal; nonfeminizing enantiomer of 17 $\beta$ -estradiol exerts protective effects in neuronal cultures and rat model of cerebral ischemia)  
IT Nerve  
(neuron; nonfeminizing enantiomer of 17 $\beta$ -estradiol exerts protective effects in neuronal cultures and rat model of cerebral ischemia)  
IT Cytoprotective agents  
(neuroprotectants; nonfeminizing enantiomer of 17 $\beta$ -estradiol exerts protective effects in neuronal cultures and rat model of cerebral ischemia)  
IT Oxidative stress, biological  
(nonfeminizing enantiomer of 17 $\beta$ -estradiol exerts protective effects in neuronal cultures and rat model of cerebral ischemia)  
IT Estrogens  
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(nonfeminizing enantiomer of 17 $\beta$ -estradiol exerts protective effects in neuronal cultures and rat model of cerebral ischemia)

IT Estrogen receptors  
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(nonfeminizing enantiomer of 17 $\beta$ -estradiol exerts protective effects in neuronal cultures and rat model of cerebral ischemia)

IT 7722-84-1, Hydrogen peroxide, biological studies  
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)  
(nonfeminizing enantiomer of 17 $\beta$ -estradiol exerts protective effects in neuronal cultures and rat model of cerebral ischemia)

IT 50-28-2, 17 $\beta$ -Estradiol, biological studies 3736-22-9  
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(nonfeminizing enantiomer of 17 $\beta$ -estradiol exerts protective effects in neuronal cultures and rat model of cerebral ischemia)

RE.CNT 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD

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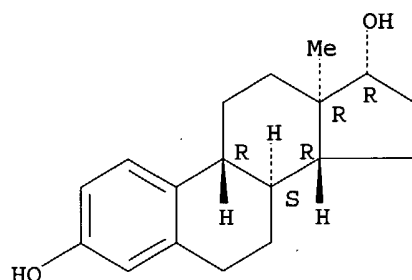
IT 3736-22-9

RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(nonfeminizing enantiomer of 17 $\beta$ -estradiol exerts protective effects in neuronal cultures and rat model of cerebral ischemia)

RN 3736-22-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, (8 $\alpha$ ,9 $\beta$ ,13 $\alpha$ ,14 $\beta$ ,17.  
alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L50 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2000:820327 HCAPLUS

DN 134:101056

ED Entered STN: 23 Nov 2000

TI Synthesis and Biological Evaluation of 17 $\beta$ -Alkoxyestra-1,3,5(10)-trienes as Potential Neuroprotectants Against Oxidative Stress

AU Prokai, Laszlo; Oon, Su-Min; Prokai-Tatrai, Katalin; Abboud, Khalil A.; Simpkins, James W.

CS Center for Drug Discovery College of Pharmacy Department of Anesthesiology College of Medicine and Center for Neurobiology of Aging College of Pharmacy, University of Florida, Gainesville, FL, 32610-0497, USA

SO Journal of Medicinal Chemistry (2001), 44(1), 110-114

CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

CC 32-3 (Steroids)

Section cross-reference(s): 1, 75

OS CASREACT 134:101056

AB 17 $\beta$ -O-Alkyl ethers (Me, Et, Pr, Bu, hexyl, and octyl) of estradiol were obtained from 3-O-benzyl-17 $\beta$ -estradiol with sodium hydride/alkyl halide, followed by the removal of the O-benzyl protecting group via catalytic transfer hydrogenation. An increase compared to estradiol in the protection of neural (HT-22) cells against oxidative stress due to exposure of glutamate was furnished by higher (C-3 to C-8) alkyl ethers, while Me and Et ethers decreased the neuroprotective effect significantly. Lipophilic (Bu and octyl) ethers blocking the phenolic hydroxyl (3-OH) of A-ring were inactive.

ST alkoxyestratriene prepn neuroprotectant oxidative stress; estratriene alkoxy prepn neuroprotectant oxidative stress

IT Cytoprotective agents

(neuroprotectants; synthesis and biol. evaluation of 17 $\beta$ -alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

IT Crystal structure

## Molecular structure

## Oxidative stress, biological

(synthesis and biol. evaluation of 17 $\beta$ -alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

## IT Estrogens

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis and biol. evaluation of 17 $\beta$ -alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

## IT 319427-05-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis and biol. evaluation of 17 $\beta$ -alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

## IT 4954-12-5P 21830-24-0P 128805-68-5P

319427-03-7P 319427-04-8P 319427-06-0P  
319427-07-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis and biol. evaluation of 17 $\beta$ -alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

IT 50-28-2, 17 $\beta$ -Estradiol, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(synthesis and biol. evaluation of 17 $\beta$ -alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

## IT 14982-15-1P 141318-37-8P 319426-98-7P

319426-99-8P 319427-00-4P 319427-01-5P  
319427-02-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and biol. evaluation of 17 $\beta$ -alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD  
RE

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IT 319427-05-9P

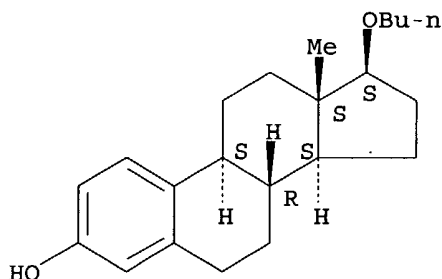
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis and biol. evaluation of 17 $\beta$ -alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

RN 319427-05-9 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-butoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 4954-12-5P 21830-24-0P 128805-68-5P

319427-03-7P 319427-04-8P 319427-06-0P

319427-07-1P

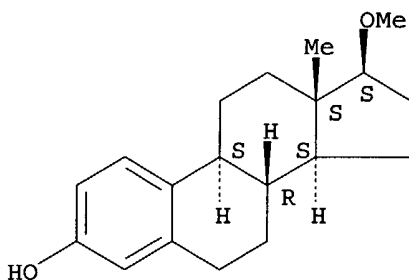
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis and biol. evaluation of 17 $\beta$ -alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

RN 4954-12-5 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

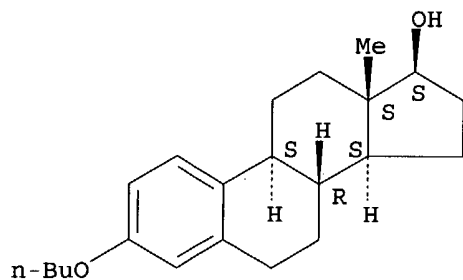
Absolute stereochemistry.



RN 21830-24-0 HCAPLUS

CN Estra-1,3,5(10)-trien-17-ol, 3-butoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

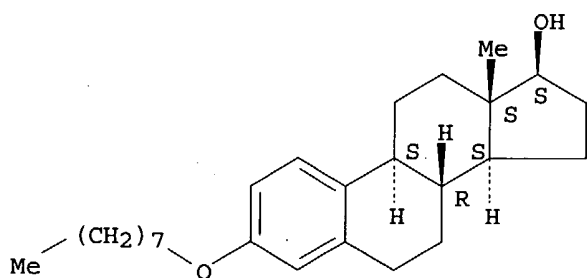
Absolute stereochemistry.



RN 128805-68-5 HCAPLUS

CN Estra-1,3,5(10)-trien-17-ol, 3-(octyloxy)-, (17β)- (9CI) (CA INDEX NAME)

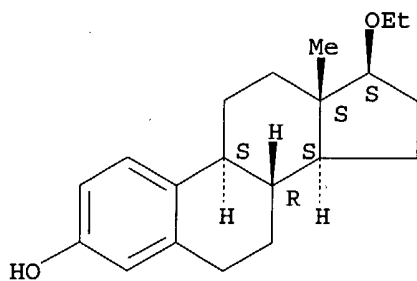
Absolute stereochemistry.



RN 319427-03-7 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-ethoxy-, (17β)- (9CI) (CA INDEX NAME)

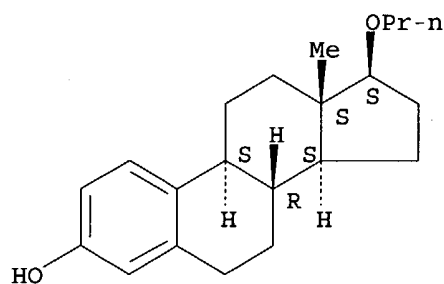
Absolute stereochemistry.



RN 319427-04-8 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-propoxy-, (17β)- (9CI) (CA INDEX NAME)

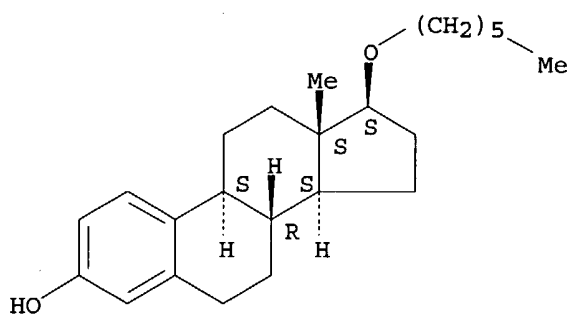
Absolute stereochemistry.



RN 319427-06-0 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-(hexyloxy)-, (17β)- (9CI) (CA INDEX NAME)

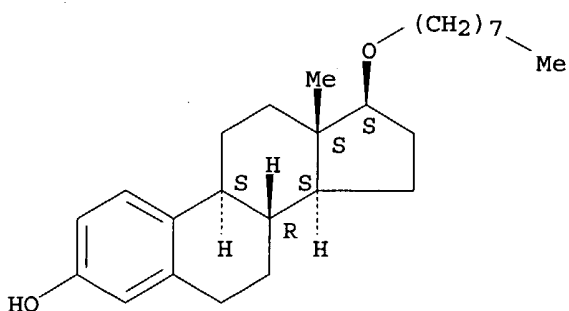
Absolute stereochemistry.



RN 319427-07-1 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-(octyloxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 14982-15-1P 141318-37-8P 319426-98-7P  
319426-99-8P 319427-00-4P 319427-01-5P  
319427-02-6P

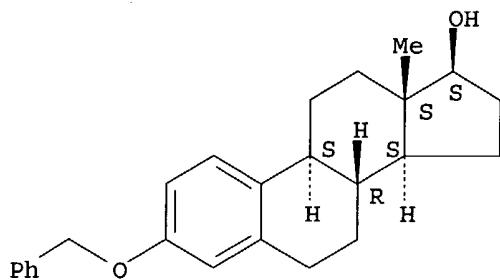
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and biol. evaluation of 17β-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

RN 14982-15-1 HCAPLUS

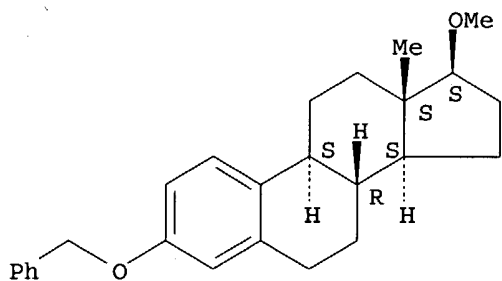
CN Estra-1,3,5(10)-trien-17-ol, 3-(phenylmethoxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



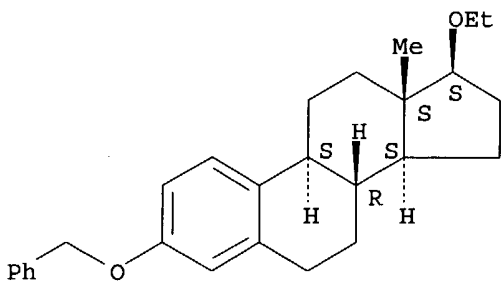
RN 141318-37-8 HCAPLUS  
 CN Estra-1,3,5(10)-triene, 17-methoxy-3-(phenylmethoxy)-, (17 $\beta$ )- (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.



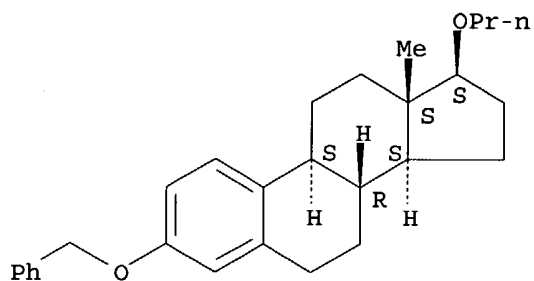
RN 319426-98-7 HCAPLUS  
 CN Estra-1,3,5(10)-triene, 17-ethoxy-3-(phenylmethoxy)-, (17 $\beta$ )- (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.



RN 319426-99-8 HCAPLUS  
 CN Estra-1,3,5(10)-triene, 3-(phenylmethoxy)-17-propoxy-, (17 $\beta$ )- (9CI)  
 (CA INDEX NAME)

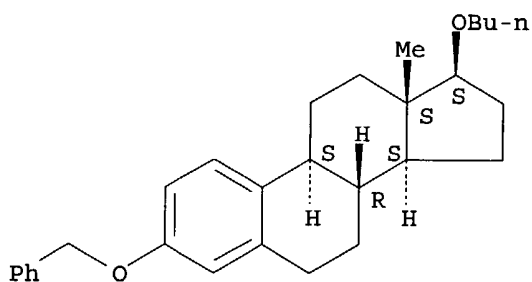
Absolute stereochemistry.



RN 319427-00-4 HCAPLUS

CN Estra-1,3,5(10)-triene, 17-butoxy-3-(phenylmethoxy)-, (17β)- (9CI)  
(CA INDEX NAME)

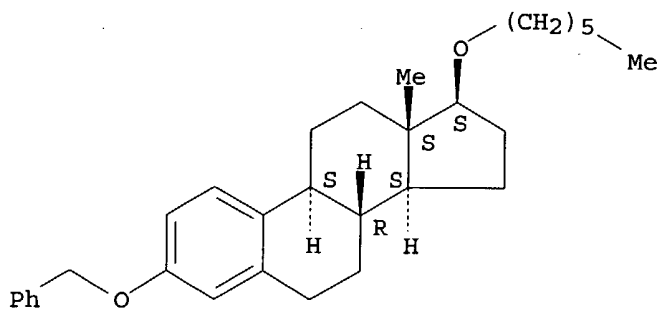
Absolute stereochemistry.



RN 319427-01-5 HCAPLUS

CN Estra-1,3,5(10)-triene, 17-(hexyloxy)-3-(phenylmethoxy)-, (17β)-  
(9CI) (CA INDEX NAME)

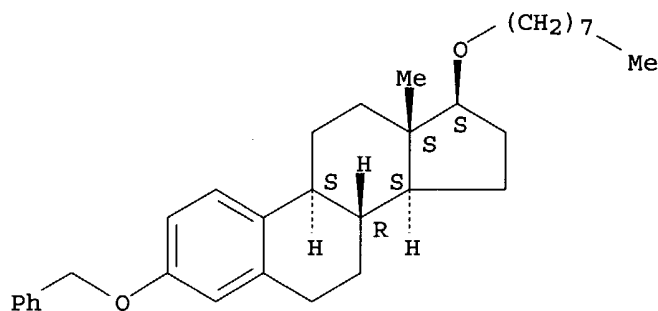
Absolute stereochemistry.



RN 319427-02-6 HCAPLUS

CN Estra-1,3,5(10)-triene, 17-(octyloxy)-3-(phenylmethoxy)-, (17β)-  
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L50 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1997:204238 HCAPLUS  
 DN 126:195255  
 ED Entered STN: 28 Mar 1997  
 TI Use of non-estrogen polycyclic phenol compounds for the manufacture of a  
 medicament for conferring neuroprotection to cells  
 IN **Simpkins, James W.**; Green, Patti S.; Gordon, Katherine  
 PA University of Florida Research Foundation, Incorporated, USA  
 SO PCT Int. Appl., 34 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 IC ICM A61K031-00  
 ICS A61K031-05; A61K031-045; A61K031-11; A61K031-12; A61K031-56  
 CC 1-11 (Pharmacology)  
 Section cross-reference(s): 2  
 FAN.CNT 9

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9703661	A1	19970206	WO 1996-US12146	19960724
	W: AU, CA, JP, KR				
	RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	CA 2227634	AA	19970206	CA 1996-2227634	19960724
	AU 9665079	A1	19970218	AU 1996-65079	19960724
	EP 841906	A1	19980520	EP 1996-924692	19960724
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	JP 11510144	T2	19990907	JP 1996-506961	19960724
	US 6197833	B1	20010306	US 1998-129209	19980804
PRAI	US 1995-1394P	P	19950724		
	US 1996-685574	A3	19960724		
	WO 1996-US12146	W	19960724		

AB Non-estrogen compds. having a terminal phenol group in a structure containing at least a second ring and having a mol. weight of less than 1000 Daltons (e.g. naphthols, phenanthrenes or steroids) are used for the manufacture of a medicament for conferring neuroprotection to cells in a subject.

ST polycyclic phenol deriv neuroprotectant

IT Nervous system

(degeneration; non-estrogen polycyclic phenol compds. for neuroprotectants)

IT Structure-activity relationship

(neuroprotectant; non-estrogen polycyclic phenol compds. for neuroprotectants)

IT Cytoprotective agents

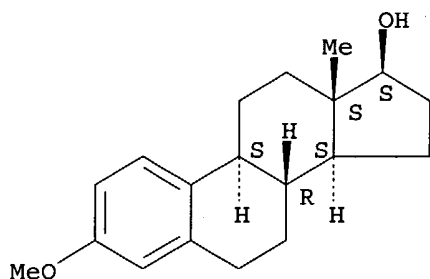
(neuroprotectants; non-estrogen polycyclic phenol compds. for neuroprotectants)

IT Anti-ischemic agents

(non-estrogen polycyclic phenol compds. for neuroprotectants)

- IT Polycyclic compounds  
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(phenols; non-estrogen polycyclic phenol compds. for neuroprotectants)
- IT Phenols, biological studies  
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(polycyclic; non-estrogen polycyclic phenol compds. for neuroprotectants)
- IT Amyloid  
RL: ADV (Adverse effect, including toxicity); BPR (Biological process);  
BSU (Biological study, unclassified); BIOL (Biological study); PROC  
(Process)  
( $\beta$ -, A $\beta$  25-35, neurotoxicity from; non-estrogen polycyclic phenol compds. for neuroprotectants)
- IT 52-39-1, Aldosterone 53-06-5, Cortisone 57-83-0, Progesterone, biological studies 57-88-5, Cholesterol, biological studies 58-22-0, Testosterone 72-33-3, Mestranol 108-95-2, Phenol, biological studies 128-37-0, Butylated hydroxytoluene, biological studies 130-79-0 521-18-6, Dihydrotestosterone 1035-77-4 1474-53-9 1624-62-0 5976-67-0 15068-98-1 25013-16-5, Butylated hydroxyanisole  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)  
(non-estrogen polycyclic phenol compds. for neuroprotectants)
- IT 50-24-8, Prednisolone 50-27-1, Estriol 50-28-2, 3,17 $\beta$ -Estradiol, biological studies 53-16-7, Estrone, biological studies 53-63-4, Estra-1,3,5(10)-trien-3-ol 56-53-1 57-63-6, 17 $\alpha$ -Ethynyl estradiol 57-91-0 83-43-2, 6 $\alpha$ -Methylprednisolone 362-05-0 18839-90-2 104849-43-6 114549-37-0  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(non-estrogen polycyclic phenol compds. for neuroprotectants)
- IT 85-01-8D, Phenanthrene, phenol group-containing derivs., biological studies 91-20-3D, Naphthalene, phenol group-containing derivs., biological studies 1321-67-1, Naphthol 29966-04-9D, Octahydrophenanthrene, phenol group-containing derivs. 51057-65-9, Phenanthrenemethanol 73493-69-3D, Tetrahydrophenanthrene, phenol group-containing derivs. 77468-40-7, Phenanthrenecarboxaldehyde  
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(non-estrogen polycyclic phenol compds. for neuroprotectants)
- IT 1035-77-4  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)  
(non-estrogen polycyclic phenol compds. for neuroprotectants)
- RN 1035-77-4 HCAPLUS
- CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AN 1996:580562 HCAPLUS  
 DN 125:294029  
 ED Entered STN: 30 Sep 1996  
 TI Methods for neuroprotection  
 IN **Simpkins, James W.**; Singh, Meharvan; Bishop, Jean  
 PA University of Florida, USA  
 SO U.S., 25 pp., Cont.-in-part of U.S. Ser. No. 149,175, abandoned.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC ICM A61K031-56  
 NCL 514182000  
 CC 2-4 (Mammalian Hormones)  
 FAN.CNT 9

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5554601	A	19960910	US 1994-318042	19941004
	CA 2175603	AA	19950511	CA 1994-2175603	19941107
	WO 9512402	A1	19950511	WO 1994-US12782	19941107
	W: AU, CA, JP, KR				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9510901	A1	19950523	AU 1995-10901	19941107
	AU 699361	B2	19981203		
	EP 799041	A1	19971008	EP 1995-901795	19941107
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
	JP 11514327	T2	19991207	JP 1994-513454	19941107
	US 5843934	A	19981201	US 1996-648857	19960516
	US 5877169	A	19990302	US 1996-749703	19961115
	US 6319914	B1	20011120	US 1999-351492	19990712
	US 2003069217	A1	20030410	US 2002-82812	20020225
PRAI	US 1993-149175	B2	19931105		
	US 1994-318042	A	19941004		
	WO 1994-US12782	W	19941107		
	US 1996-648857	A2	19960516		
	US 1996-685574	A2	19960724		
	US 1996-749703	A3	19961115		
	US 1997-782883	A3	19970110		
	US 1998-128862	A3	19980804		
	US 1998-129209	A2	19980804		
	US 1998-179640	A3	19981027		
	US 1999-372627	A1	19990811		
AB	A method is provided for conferring neuroprotection on a population of cells using estrogen compds. that have insubstantial sex activity and furthermore, a method is provided that utilizes estrogen compds. in the absence of testosterone for treating neurodegenerative diseases including Alzheimer's disease to retard the adverse effects of these disorders, Examples of estrogen compds. that have insubstantial sex activity includes alpha isomers of estrogen compds. such as 17 $\alpha$ -estradiol.				
ST	estrogen neuroprotection				
IT	Nerve				
	(methods for neuroprotection)				
IT	Estrogens				
	RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)				
	(methods for neuroprotection)				
IT	Molecular structure-biological activity relationship				
	(neuroprotective; methods for neuroprotection)				
IT	Mental disorder				
	(Alzheimer's disease, methods for neuroprotection)				
IT	53-16-7, biological studies 57-63-6, 17 $\alpha$ -Ethinylestradiol				
	57-91-0, 17 $\alpha$ -Estradiol 10093-54-6 15068-99-2 33602-53-8				
	65684-87-9 110114-70-0 182624-49-3 182624-50-6				
	182624-51-7 182624-52-8 182624-53-9 182624-54-0				
	182624-55-1 182624-56-2 182624-57-3 182624-58-4 182624-59-5				

182624-60-8 182624-61-9 182823-27-4

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(methods for neuroprotection)

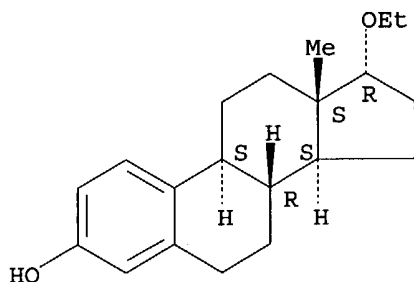
IT 182624-49-3 182624-51-7 182823-27-4

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(methods for neuroprotection)

RN 182624-49-3 HCAPLUS

CN Estradiol, 17-ethoxy-, (17 $\alpha$ )- (9CI) (CA INDEX  
NAME)

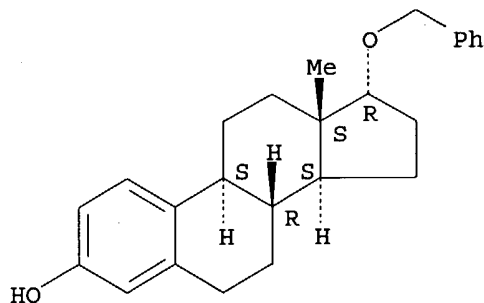
Absolute stereochemistry.



RN 182624-51-7 HCAPLUS

CN Estradiol, 17-(phenylmethoxy)-, (17 $\alpha$ )- (9CI) (CA  
INDEX NAME)

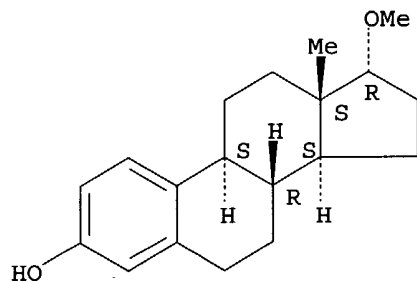
Absolute stereochemistry.



RN 182823-27-4 HCAPLUS

CN Estradiol, 17-methoxy-, (17 $\alpha$ )- (9CI) (CA INDEX  
NAME)

Absolute stereochemistry.



AN 1988:623419 HCAPLUS  
 DN 109:223419  
 ED Entered STN: 24 Dec 1988  
 TI Preparation and use of brain-specific dihydropyridine redox carrier-type derivatives of estrogenic agents for treating male sexual dysfunction  
 IN Anderson, Wesley R.; Bodor, Nicholas S.; Simpkins, James W.  
 PA University of Florida, USA  
 SO Eur. Pat. Appl., 60 pp.  
 CODEN: EPXXDW  
 DT Patent  
 LA English  
 IC ICM A61K031-565  
 ICA A61K031-44  
 CC 2-10 (Mammalian Hormones)  
 Section cross-reference(s): 27

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 256668	A2	19880224	EP 1987-306224	19870714
	EP 256668	A3	19891004		
	EP 256668	B1	19921104		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	US 4863911	A	19890905	US 1986-892861	19860804
	AT 81977	E	19921115	AT 1987-306224	19870714
	AU 8776308	A1	19880211	AU 1987-76308	19870730
	AU 603368	B2	19901115		
	CA 1300020	A1	19920505	CA 1987-543611	19870803
	JP 63099095	A2	19880430	JP 1987-195140	19870804
	JP 2646568	B2	19970827		
PRAI	US 1986-892861		19860804		
	EP 1987-306224		19870714		

OS MARPAT 109:223419

AB Compds. E-DHC or E-[DHC]<sub>n</sub> [E = estrogen or estrogen with reactive OH group(s); DHC = reduced, biooxidizable, blood-brain barrier-penetrating, lipoidal form of a dihydropyridine-pyridinium salt redox carrier; n = number of reactive OH groups] or nontoxic pharmaceutically acceptable salts are used to prepare a medication for treating male sexual dysfunction. 17 $\beta$ -[(1-Methyl-1,4-dihydro-3-pyridinyl)carbonyloxy]estra-1,3,5(10)-trien-3-ol (I) was prepared from estradiol and nicotinoyl chloride hydrochloride in 4 steps. Bilaterally orchidectomized adult male Sprague-Dawley rats were injected with I (3 mg/kg in DMSO). The animals responded with a decrease in mounting and intromission latencies by 3 days which persisted for >28 days. Intromission frequencies increased by 300% over castrate levels through 14 days and were restored to precastrate levels through 4 wk.

ST estrogen dihydropyridine conjugate male sexual dysfunction

IT Steroids, compounds

RL: BIOL (Biological study)

(1,3,5(10)-triunsatd., hydroxy, conjugates, with dihydropyridine redox carriers, for treating male sexual dysfunction)

IT Sex

(activity, disorder, male, treatment of, by estrogen-dihydropyridine redox carrier conjugates)

IT Estrogens

RL: BIOL (Biological study)

(conjugates, with dihydropyridine redox carriers, for treatment of male sexual dysfunction)

IT 50-27-1D, Estriol, dihydropyridine redox carrier conjugates 50-28-2D, Estradiol, dihydropyridine redox carrier conjugates 50-50-0D, Estradiol benzoate, dihydropyridine redox carrier conjugates 53-16-7D, Estrone, dihydropyridine redox carrier conjugates 57-63-6D, Ethinyl estradiol, dihydropyridine redox carrier conjugates 72-33-3D, Mestranol, dihydropyridine redox carrier conjugates 152-43-2D, Quinestrol,

dihydropyridine redox carrier conjugates 313-06-4D, Estradiol cypionate,  
 dihydropyridine redox carrier conjugates 979-32-8D, Estradiol valerate,  
 dihydropyridine redox carrier conjugates 3571-53-7D, Estradiol  
 undecylate, dihydropyridine redox carrier conjugates 3758-34-7D,  
 dihydropyridine redox carrier conjugates 4956-37-0D, Estradiol  
 enanthate, dihydropyridine redox carrier conjugates 5941-36-6D,  
 Estrazinol, dihydropyridine redox carrier conjugates 10322-73-3D,  
 dihydropyridine redox carrier conjugates 27790-75-6D, Dihydropyridine,  
 derivs., estrogen conjugates 39791-20-3D, Nylestriol, dihydropyridine  
 redox carrier conjugates 47703-84-4D, dihydropyridine redox carrier  
 conjugates 117539-14-7D, estrogens conjugates

RL: BIOL (Biological study)

(male sexual dysfunction treatment by)

IT 4248-62-8P 4248-63-9P 20260-53-1P, Nicotinoyl chloride hydrochloride  
 104117-66-0P 106146-62-7P 106146-63-8P 106146-65-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)

(preparation and reaction of, in preparation of estrogen-dihydropyridine

redox

carrier conjugates for treating male sexual dysfunction)

IT 103562-82-9P

RL: PREP (Preparation)

(preparation of and male sexual dysfunction treatment by)

IT 106146-61-6P 106146-64-9P 106146-66-1P 106146-67-2P

RL: PREP (Preparation)

(preparation of, for treating male sexual dysfunction)

IT 50-28-2, Estradiol, reactions 53-16-7, Estrone, reactions 59-67-6,

Nicotinic acid, reactions 1035-77-4, Estradiol-3-methyl ether

7719-09-7, Thionyl chloride 117539-15-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in preparation of estrogen-dihydropyridine redox carrier  
 conjugates for treating male sexual dysfunction)

IT 1035-77-4, Estradiol-3-methyl ether

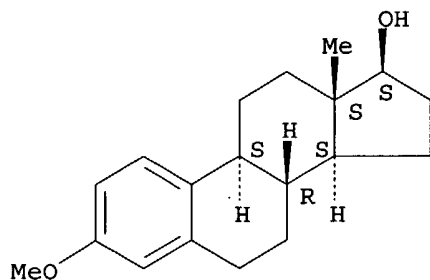
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in preparation of estrogen-dihydropyridine redox carrier  
 conjugates for treating male sexual dysfunction)

RN 1035-77-4 HCAPLUS

CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX  
 NAME)

Absolute stereochemistry.



L50 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1987:27813 HCAPLUS

DN 106:27813

ED Entered STN: 07 Feb 1987

TI Method and compositions for weight control

IN Bodor, Nicholas S.; Estes, Kerry S.; Simpkins, James W.

PA University of Florida, USA

SO U.S., 33 pp.

CODEN: USXXAM

DT Patent

LA English

IC ICM A61K031-58

NCL 514176000

CC 1-10 (Pharmacology)

Section cross-reference(s): 32

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4617298	A	19861014	US 1985-790159	19851022
	AU 8663425	A1	19870430	AU 1986-63425	19861001
	EP 220844	A2	19870506	EP 1986-307536	19861001
	EP 220844	A3	19890830		

R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE

PRAI US 1985-790159 19851022

OS CASREACT 106:27813

AB A method is given for controlling mammalian body weight by administration of E-DHC where E is an estrogen and DHC is the reduced, biooxidizable, blood-brain barrier penetrating, lipoidal form of a dihydropyridine.dblarw.pyridinium salt redox carrier. A preferred compound is the estrdiol derivative 17 $\beta$ -[(1-methyl-1,4-dihydro-3-pyridinyl)carbonyloxy]estra-1,3,5(10)-trien-3-ol (I). Thus, administration of 1-5 mg I/kg to female rats caused weight loss with little effect on the estrous cycle. The synthesis of the compds. is given.

ST estrogen pyridinyl prepn antiobesity agent

IT Estrogens

RL: BIOL (Biological study)

(dihydropyridine redox-type derivs., as antiobesity agents)

IT Antiobesity agents

(estrogen dihydropyridine redox-type derivs.)

IT 59-67-6, Nicotinic acid, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(esterification by, of estrone via acid chloride)

IT 50-28-2, biological studies 53-16-7, Estrone, reactions

1035-77-4, Estradiol 3-methyl ether

RL: RCT (Reactant); RACT (Reactant or reagent)

(esterification of, with nicotinoyl chloride)

IT 106146-62-7P 106146-63-8P 106146-64-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and dithionite reduction of)

IT 20260-53-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and esterification by, of estrogens)

IT 4248-62-8P 4248-63-9P 104117-66-0P 106146-65-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and quaternization of, with Me iodide)

IT 106146-61-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and selective hydrolysis of)

IT 106146-66-1P 106146-67-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as body weight-reducing agent)

IT 103562-82-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, with body weight-reducing agent)

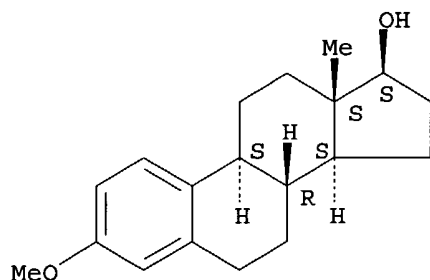
IT 74-88-4, Methyl iodide, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(quaternization by, of estrone nicotinate)

IT 1035-77-4, Estradiol 3-methyl ether  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (esterification of, with nicotinoyl chloride)  
 RN 1035-77-4 HCAPLUS  
 CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> => d all hitstr tot 159

L59 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2002:974249 HCAPLUS  
 DN 138:44718  
 ED Entered STN: 26 Dec 2002  
 TI Extended-release growth promoting two component composition  
 IN Cady, Susan Mancini; Macar, Claude; Gibson, John W.  
 PA Akzo Nobel N.V., Neth.; Southern Biosystems  
 SO U.S., 10 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC ICM A61K031-56  
 ICS A61K031-335; C07J001-00; C07D313-08  
 NCL 514170000; 514171000; 514178000; 514182000; 514450000; 552625000;  
 552646000; 552650000; 549269000  
 CC 63-6 (Pharmaceuticals)  
 Section cross-reference(s): 18

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6498153	B1	20021224	US 1999-273862	19990322 <--
PRAI	FR 1998-16707	A	19981231	<--	
OS	MARPAT 138:44718				

AB An extended-release composition comprising a first composition comprising growth promoters and a second composition comprising growth promoters and a biodegradable polymer is described. A method of increasing weight gain in food animals utilizing the composition, a pharmaceutical dosage form containing the composition and a method of preparing the pharmaceutical dosage form are also described, as are pellets of the composition for implantation in food animals. For example, 1000 g of a mixture of 17 $\beta$ -acetoxy-4,9,11-trien-3-one and estra-1,3,5(10)-trien-3,17 $\beta$ -diol, also containing cholesterol, Et cellulose and magnesium stearate, was granulated with 52.6 g of 75:25 DL-lactide-glycolide copolymer. The dried, sieved granulation was tableted to provide pellets with an average weight of about 33 mg and an average hardness of about 70 N. Pellets were then coated with

- DL-lactide-glycolide copolymer (65:25 or 75:25, resp.).
- ST growth promoter biodegradable polymer pellet controlled release implant;  
farm animal growth promoter controlled release implant
- IT Polymers, biological studies  
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(biodegradable; pellets containing growth promoters and biodegradable polymers for controlled-release implants for farm animals)
- IT Polyesters, biological studies  
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(dilactone-based; pellets containing growth promoters and biodegradable polymers for controlled-release implants for farm animals)
- IT Polyesters, biological studies  
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(glycolide-based; pellets containing growth promoters and biodegradable polymers for controlled-release implants for farm animals)
- IT Drug delivery systems  
(implants, controlled-release; pellets containing growth promoters and biodegradable polymers for controlled-release implants for farm animals)
- IT Polyesters, biological studies  
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(lactide; pellets containing growth promoters and biodegradable polymers for controlled-release implants for farm animals)
- IT Glass transition temperature  
Livestock  
(pellets containing growth promoters and biodegradable polymers for controlled-release implants for farm animals)
- IT Growth factors, animal  
RL: AGR (Agricultural use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(pellets containing growth promoters and biodegradable polymers for controlled-release implants for farm animals)
- IT Drug delivery systems  
(pellets; pellets containing growth promoters and biodegradable polymers for controlled-release implants for farm animals)
- IT 50-28-2, Estra-1,3,5(10)-triene-3,17-diol (17 $\beta$ )-, biological studies  
57-83-0, Pregn-4-ene-3,20-dione, biological studies 57-85-2,  
17 $\beta$ -Propionyloxy-4-androsten-3-one 10109-77-0 10161-34-9,  
17 $\beta$ -Acetoxystestra-4,9,11-trien-3-one 55331-29-8 55561-42-7  
RL: AGR (Agricultural use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(pellets containing growth promoters and biodegradable polymers for controlled-release implants for farm animals)
- IT 26009-03-0, Polyglycolide 26023-30-3, Poly[oxy(1-methyl-2-oxo-1,2-ethanediyl)] 26161-42-2 26202-08-4, Polyglycolide 26680-10-4,  
Poly(DL-lactide) 26780-50-7, Glycolide-DL-lactide copolymer  
30846-39-0, Glycolide-L-lactide copolymer 33135-50-1, Poly(L-lactide)  
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(pellets containing growth promoters and biodegradable polymers for controlled-release implants for farm animals)

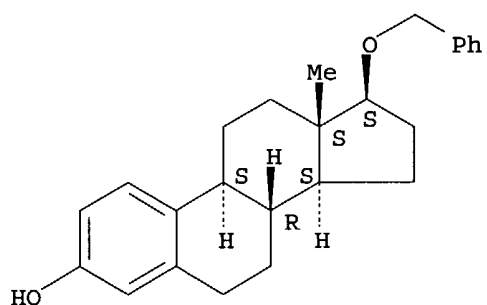
RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Anon; GB 2167662 A 1986 HCAPLUS
- (2) Boswell; US 3773919 A 1973 HCAPLUS
- (3) Brown; US 4393041 A 1983 HCAPLUS
- (4) Deasy, P; International Journal of Pharmaceutics 1993, V89, P251 HCAPLUS
- (5) Dirix; US 5389379 A 1995 HCAPLUS
- (6) Foutz, C; Journal of Animal Science 1997, V75, P1256 HCAPLUS
- (7) Grandadam; US 3939265 A 1976 HCAPLUS
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- (9) Herbert; US 5654008 A 1997 HCAPLUS
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 IT 55561-42-7  
 RL: AGR (Agricultural use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (pellets containing growth promoters and biodegradable polymers for controlled-release implants for farm animals)  
 RN 55561-42-7 HCAPLUS  
 CN Estradiol, 17-(phenylmethoxy)-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1999:30570 HCAPLUS  
 DN 130:293190  
 ED Entered STN: 15 Jan 1999  
 TI Human 17 $\beta$ -hydroxysteroid dehydrogenase-ligand complexes: crystals of different space groups with various cations and combined seeding and co-crystallization  
 AU Zhu, D.-W.; Han, Q.; Qiu, W.; Campbell, R. L.; Xie, B.-X.; Azzi, A.; Lin, S.-X.  
 CS CHUL Research Center, Medical Research Council Group in Molecular Endocrinology, Laval University, Quebec, G1V 4G2, Can.  
 SO Journal of Crystal Growth (1999), 196(2-4), 356-364  
 CODEN: JCRGAE; ISSN: 0022-0248  
 PB Elsevier Science B.V.  
 DT Journal  
 LA English  
 CC 7-5 (Enzymes)  
 Section cross-reference(s): 75  
 AB Human estrogenic 17 $\beta$ -hydroxysteroid dehydrogenase (17 $\beta$ -HSD1) is responsible for the synthesis of active estrogens that stimulate the proliferation of breast cancer cells. The enzyme has been crystallized using a Mg<sup>2+</sup>/PEG (3500)/ $\beta$ -octyl glucoside system. The space group of these crystals is C2. Here we report that cations can affect 17 $\beta$ -HSD1 crystallization significantly. In the presence of Mn<sup>2+</sup> instead of Mg<sup>2+</sup>, crystals have been obtained in the same space group with similar unit cell dimensions. In the presence of Li<sup>+</sup> and Na<sup>+</sup> instead of Mg<sup>2+</sup>, the space group has been changed to P212121. A whole data set for a crystal of 17 $\beta$ -HSD1 complex with progesterone grown in the presence of Li<sup>+</sup> has been collected to 1.95 Å resolution with a synchrotron source. The cell dimensions are a=41.91 Å, b=108.21 Å, c=117.00 Å. The structure has been preliminarily determined by mol. replacement, yielding

important information on crystal packing in the presence of different cations. In order to further understand the structure-function relationship of 17 $\beta$ -HSD1, enzyme complexes with several ligands have been crystallized. As the steroids have very low aqueous solubility, we used a combined

method of seeding and co-crystallization to obtain crystals of 17 $\beta$ -HSD1 complexed with various ligands. This method provides ideal conditions for growing complex crystals, with ligands such as 20 $\alpha$ -hydroxysteroid progesterone, testosterone and 17 $\beta$ -methyl-estradiol-NADP+. Several complex structures have been determined with reliable electronic d. of the bound ligands.

ST hydroxysteroid dehydrogenase ligand complex human; crystal structure hydroxysteroid dehydrogenase ligand complex human

IT Cations

Crystal growth

Crystal structure

(crystals of human 17 $\beta$ -hydroxysteroid dehydrogenase-ligand complexes have different space groups with various cations)

IT 9028-61-9, 17 $\beta$ -Estradiol dehydrogenase

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(crystals of human 17 $\beta$ -hydroxysteroid dehydrogenase-ligand complexes have different space groups with various cations)

IT 53-59-8DP, Nadp, complexes with 17 $\beta$ -hydroxysteroid dehydrogenase and 17 $\beta$ -methylestradiol 58-22-0DP, Testosterone, complexes with 17 $\beta$ -hydroxysteroid dehydrogenase 145-14-2DP, 20 $\alpha$ -

HydroxyProgesterone, complexes with 17 $\beta$ -hydroxysteroid dehydrogenase 4954-12-5DP, complexes with 17 $\beta$ -hydroxysteroid dehydrogenase

and NADP 9028-61-9DP, 17 $\beta$ -Estradiol dehydrogenase, ligand complexes

RL: PNU (Preparation, unclassified); PRP (Properties); PREP (Preparation)

(crystals of human 17 $\beta$ -hydroxysteroid dehydrogenase-ligand complexes have different space groups with various cations)

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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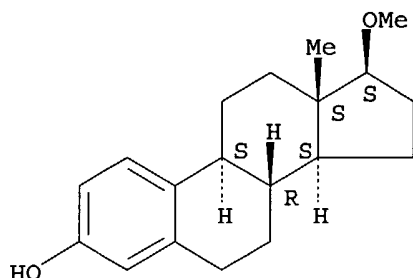
IT 4954-12-5DP, complexes with 17 $\beta$ -hydroxysteroid dehydrogenase and NADP

RL: PNU (Preparation, unclassified); PRP (Properties); PREP (Preparation)  
(crystals of human 17 $\beta$ -hydroxysteroid dehydrogenase-ligand  
complexes have different space groups with various cations)

RN 4954-12-5 HCAPLUS

CN Estradiol, 17-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX  
NAME)

Absolute stereochemistry.



L59 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1998:397783 HCAPLUS

DN 129:54482

ED Entered STN: 29 Jun 1998

TI Preparation of steroid inhibitors of estrone sulfatase and associated  
pharmaceutical compositions and methods of use

IN Tanabe, Masato; Peters, Richard H.; Chao, Wan-ru; Shigeno, Kazuhiko

PA SRI International, USA

SO U.S., 23 pp.

CODEN: USXXAM

DT Patent

LA English

IC ICM A61K031-58

ICS C07J071-00

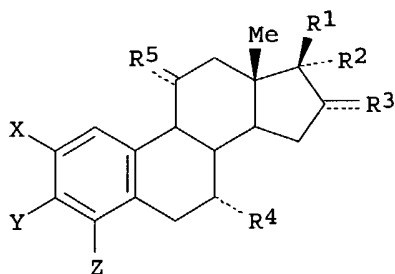
NCL 514176000

CC 32-3 (Steroids)

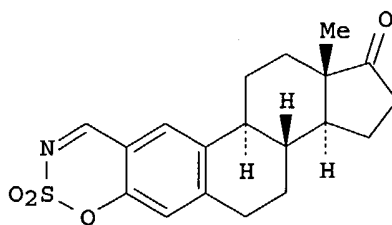
Section cross-reference(s): 1, 2

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5763432	A	19980609	US 1997-794229	19970129 <--
	US 5861388	A	19990119	US 1997-1601	19971231 <--
	WO 9832763	A1	19980730	WO 1998-US1846	19980129 <--
	W: CA, JP, KR				
	RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
PRAI	US 1997-794229		19970129	<--	
OS	MARPAT 129:54482				
GI					



I



II

AB Estratriene derivs. of formula I [X and Y, or Y and Z, form an oxathiazine dioxide ring or a dihydro-oxathiazine dioxide ring; R1, R2 = H, alkyl, alkynyl, (substituted) OH; R1R2 = O, S, (substituted) CH2; R3 = H, halo, alkyl, CH2; R4 = H, alkyl; R5 = H, OH, alkyl, alkenyl, alkoxy, aryl, CH2] are prepared as inhibitors of estrone sulfatase. Pharmaceutical compns. and methods for using I to treat estrogen-dependent disorders are provided as well. Thus, estradiol is transformed into II in 3 steps. In an estrone sulfatase inhibition assay, II showed 5-% inhibition at 9.3 nM.

ST estratriene deriv prepn estrone sulfatase inhibitor

IT 208758-20-7P 208758-22-9P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (preparation of steroid inhibitors of estrone sulfatase)

IT 208758-16-1P 208758-17-2P 208758-21-8P 208758-23-0P 208758-25-2P  
 208758-33-2P 208758-34-3P 208758-35-4P 208758-36-5P 208758-37-6P  
 208758-38-7P 208758-39-8P 208758-41-2P 208758-43-4P 208758-48-9P  
 208758-52-5P 208758-54-7P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of steroid inhibitors of estrone sulfatase)

IT 59298-96-3, Estrone sulfatase  
 RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)  
 (preparation of steroid inhibitors of estrone sulfatase)

IT 50-28-2, Estradiol, reactions 53-16-7, Estrone, reactions 57-63-6, 17 $\alpha$ -Ethinylestradiol 1530-32-1, Ethyltriphenylphosphonium bromide 1779-51-7, Butyltriphenylphosphonium bromide 4954-12-5 6228-47-3, Propyltriphenylphosphonium bromide 7678-95-7 59077-04-2, 19-Norpregna-1,3,5(10)-trien-3-ol  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of steroid inhibitors of estrone sulfatase)

IT 4736-62-3P 6599-97-9P 13879-55-5P 13879-56-6P 31559-62-3P  
 34111-53-0P 57711-40-7P 64215-82-3P 99898-93-8P 120574-27-8P  
 120574-28-9P 123715-79-7P 137352-12-6P 206442-55-9P 208758-18-3P  
 208758-19-4P 208758-24-1P 208758-26-3P 208758-27-4P 208758-28-5P  
 208758-29-6P 208758-30-9P 208758-31-0P 208758-32-1P 208758-40-1P  
 208758-42-3P 208758-44-5P 208758-45-6P 208758-46-7P 208758-47-8P  
 208758-50-3P 208758-51-4P 208758-53-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of steroid inhibitors of estrone sulfatase)

IT 208758-49-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of steroid inhibitors of estrone sulfatase)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD

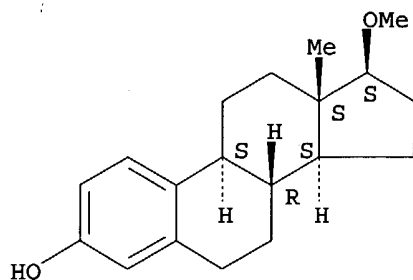
RE  
 (1) Babcock; US 4297350 1981 HCAPLUS  
 (2) Kuehne; US 3033860 1962 HCAPLUS

IT 4954-12-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of steroid inhibitors of estrone sulfatase)

RN 4954-12-5 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

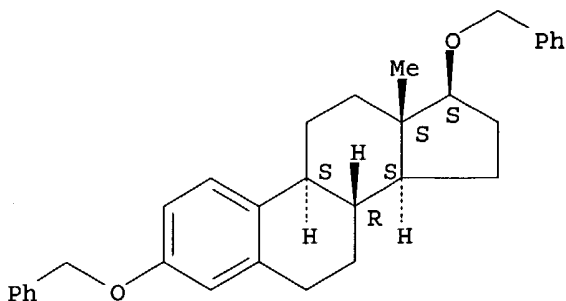
Absolute stereochemistry.



L59 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1992:570477 HCAPLUS  
 DN 117:170477  
 ED Entered STN: 01 Nov 1992  
 TI Aluminum chloride - N,N-dimethylaniline: a novel benzyl and allyl ether cleavage reagent  
 AU Akiyama, Takahiko; Hirofuji, Hajimu; Ozaki, Shoichiro  
 CS Fac. Eng., Ehime Univ., Matsuyama, 790, Japan  
 SO Bulletin of the Chemical Society of Japan (1992), 65(7), 1932-8  
 CODEN: BCSJA8; ISSN: 0009-2673  
 DT Journal  
 LA English  
 CC 21-2 (General Organic Chemistry)  
 OS CASREACT 117:170477  
 AB A combination system of AlCl<sub>3</sub>-N,N-dimethylaniline was found to cleave benzyl ethers readily to give parent alcs. in excellent yields. The system also cleaved allyl as well as Me ethers. Numerous functional groups such as benzyloxy, phenylthio, and olefinic double bond were not affected. Comparisons of AlCl<sub>3</sub>-N,N-dimethylaniline and AlCl<sub>3</sub>-anisole were described.  
 ST aluminum trichloride dimethylaniline cleavage ether; benzyl ether cleavage aluminum trichloride dimethylaniline; allyl ether cleavage aluminum trichloride dimethylaniline; aniline dimethyl aluminum trichloride cleavage ether  
 IT Ethers, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (allyl, cleavage of, with aluminum chloride and dimethylaniline)  
 IT Ethers, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (benzyl, cleavage of, with aluminum trichloride and dimethylaniline)  
 IT 78-89-7, 2-Chloro-1-propanol 4799-68-2, 3-(Benzyloxy)-1-propanol  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (benzylation of)  
 IT 2550-26-7, 4-Phenyl-2-butanone  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (borohydride reduction of)  
 IT 121-69-7, N,N-Dimethylaniline, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cleavage by aluminum trichloride and, benzyl and allyl ethers)  
 IT 100-66-3, Anisole, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cleavage by aluminum trichloride and, of benzyl and allyl ethers)  
 IT 108-95-2, Phenol, reactions 701-56-4, p-Methoxy-N,N-dimethylaniline  
 15799-79-8, m-Methoxy-N,N-dimethylaniline  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cleavage by aluminum trichloride and, of benzyl phenylpropyl ether)  
 IT 7646-78-8, Tin tetrachloride, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cleavage by anisole and, of benzyl phenylpropyl ether)

- IT 7446-70-0, Aluminum trichloride, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cleavage by dimethylaniline and, of benzylallyl ethers)
- IT 1981-90-4 67685-90-9 108741-19-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(ether cleavage of, with aluminum trichloride and dimethylaniline)
- IT 100-02-7, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(etherification of, with benzyl chloropropyl ether)
- IT 70770-06-8P, Benzyl 3-phenylpropyl ether  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and cleavage of, with aluminum trichloride and dimethylaniline)
- IT 2046-33-5P, Methyl 3-phenylpropyl ether 6793-92-6P, Benzyl 4-bromophenyl ether 7278-60-6P 64740-44-9P **69455-04-5P** 69483-57-4P 93981-51-2P 96154-40-4P 101747-16-4P 133992-66-2P 143703-94-0P 143703-95-1P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and ether cleavage of, with aluminum trichloride and dimethylaniline)
- IT 122-97-4P, 3-Phenylpropanol  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and etherification of)
- IT 50-28-2P, Estra-1,3,5(10)-triene-3,17-diol (17 $\beta$ )-, preparation 57-88-5P, Cholest-5-en-3-ol (3 $\beta$ )-, preparation 80-97-7P 106-22-9P 106-41-2P 834-14-0P 883-90-9P 2344-70-9P 2722-36-3P, 3-Phenyl-1-butanol 3204-68-0P 6946-99-2P 24536-40-1P **55561-42-7P** 66971-02-6P 104330-36-1P 131335-38-1P 131432-84-3P 143703-96-2P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)
- IT 26420-79-1P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation, etherification of, with nitrophenol and phenylsulfenylation of)
- IT **69455-04-5P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and ether cleavage of, with aluminum trichloride and dimethylaniline)
- RN 69455-04-5 HCAPLUS  
CN Estra-1,3,5(10)-triene, 3,17-bis(phenylmethoxy)-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

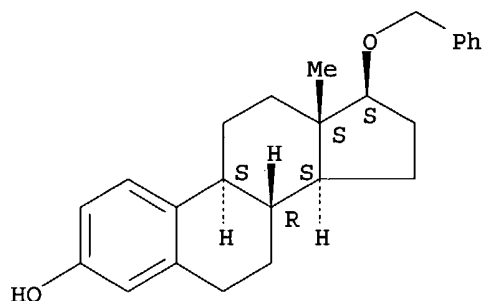
Absolute stereochemistry.



- IT **55561-42-7P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)
- RN 55561-42-7 HCAPLUS  
CN Estra-1,3,5(10)-triene-3-ol, 17-(phenylmethoxy)-, (17 $\beta$ )- (9CI) (CA

INDEX NAME)

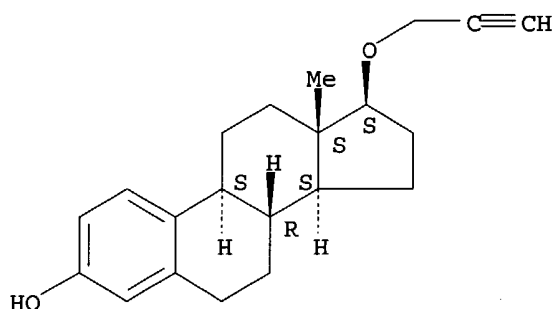
Absolute stereochemistry.



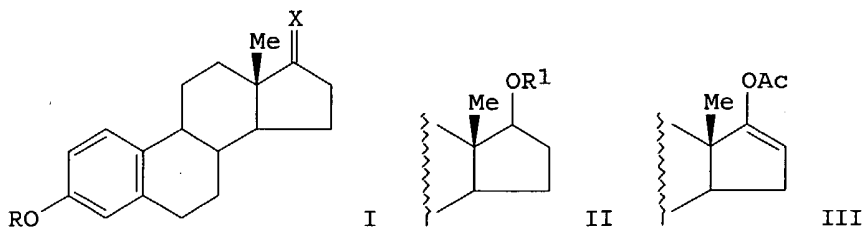
L59 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1992:408261 HCAPLUS  
 DN 117:8261  
 ED Entered STN: 11 Jul 1992  
 TI Synthesis of o-carboranylmethyl ethers of steroids as potential target substrates for boron neutron capture therapy  
 AU Schneiderova, Lenka; Strouf, Oldrich; Gruner, Bohumir; Pouzar, Vladimir; Drasar, Pavel; Hampl, Richard; Kimlova, Irena  
 CS Int. Inorg. Chem., Czech. Acad. Sci., Prague, 160 00, Czech.  
 SO Collection of Czechoslovak Chemical Communications (1992), 57(3), 463-71  
 CODEN: CCCCAK; ISSN: 0010-0765  
 DT Journal  
 LA English  
 CC 32-3 (Steroids)  
 AB o-Carboranylmethyl ethers of steroids were synthesized by insertion of steroidal 2-propynyloxy derivs. into 6,9-bis(acetonitrile)decaborane(12). This reaction afforded compds. with estrane and androstane skeleton, potentially useful in boron neutron capture therapy of hormone-sensitive forms of cancer, i.e., 17 $\beta$ -o-carboranylmethyl ether of estradiol (I) (yield 14%) and 3 $\beta$ - and 17 $\beta$ -carboranylmethyl ethers of androstenediol (yield 12% and 13%, resp.). Jones oxidation afforded carboranyl derivative of androsten-17-one in 75% yield. As shown by a study of the insertion reaction of 3 $\beta$ -(2-propynyloxy)cholest-5-ene, the low yields of the insertion reaction cannot be increased by changing the reaction conditions. The relative binding affinity of I to estrogen receptors from rat uterine and human breast tumor cytosol was 3.0 and 0.29% resp., of that of estradiol.  
 ST carboranylmethyl ether steroid; estrogen receptor binding  
 carboranylmethoxyestrol  
 IT Receptors  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (estrogen, binding by, of estradiol carboranylmethyl ether)  
 IT Estrogens  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (receptors, binding by, of estradiol carboranylmethyl ether)  
 IT 141887-27-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and binding of, to estrogen receptors)  
 IT 141870-63-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and oxidation of)  
 IT 138473-74-2P 141870-64-6P 141887-25-4P 141887-26-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)  
 IT 126003-29-0 126003-37-0 126003-41-6 **126003-44-9**  
 126003-45-0  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with carborane derivative)  
 IT 17702-41-9, Decaborane(14) 28377-97-1 32124-79-1  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with hydroxy steroid)  
 IT **126003-44-9**  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with carborane derivative)  
 RN 126003-44-9 HCAPLUS  
 CN Estr-1,3,5(10)-trien-3-ol, 17-(2-propynyloxy)-, (17 $\beta$ )- (9CI) (CA  
 INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1992:235946 HCAPLUS  
 DN 116:235946  
 ED Entered STN: 13 Jun 1992  
 TI Synthesis and properties of 3,17-disubstituted estrogenic steroids  
 AU Tong, Z. S.; Gan, G. Z.; Li, L.; Tang, Z. M.  
 CS Inst. Radiat. Med., Acad. Mil. Med. Sci., Beijing, 100850, Peop. Rep.  
 China  
 SO Yaoxue Xuebao (1992), 27(3), 236-40  
 CODEN: YHHPAL; ISSN: 0513-4870  
 DT Journal  
 LA Chinese  
 CC 32-3 (Steroids)  
 Section cross-reference(s): 8  
 GI



AB Ten title radioprotective estrogens, e.g., I [R = H, Me, cyclopentyl; X = NOME, N(CH<sub>2</sub>)<sub>n</sub>CH<sub>2</sub>OH, n = 1, 2], II (R<sub>1</sub> = H, Me, CH<sub>2</sub>CH<sub>2</sub>OH) and III were prepared I [R = cyclopentyl, X = N(CH<sub>2</sub>)<sub>n</sub>CH<sub>2</sub>OH, N = 1, 2] showed better protective effect in mice than estradiol upon 750 rad  $\gamma$ -irradiation with

60Co. Several compds. increased 30-day survival rate by 35-80% in mice exposed to 900 rad of irradiation when administered i.p. 0.1 mg per mouse 24 h before irradiation

ST estratrienol prepn radioprotectant

IT Radioprotectants  
(estratrienols, against  $\gamma$ -rays)

IT **141318-37-8P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and debenzylation of)

IT **14982-15-1P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and methylation of)

IT 2774-51-8P **4954-12-5P** 6038-28-4P 27543-03-9P 94514-10-0P  
94514-11-1P 94514-13-3P 94514-15-5P 94876-43-4P 97117-16-3P  
141276-94-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and radioprotective activity of)

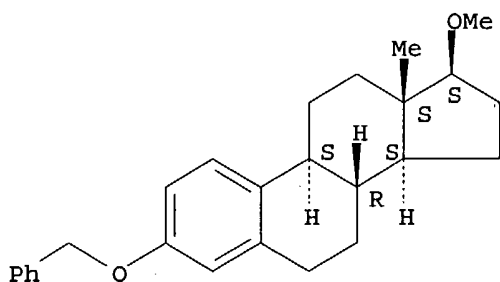
IT **141318-37-8P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and debenzylation of)

RN 141318-37-8 HCAPLUS

CN Estra-1,3,5(10)-triene, 17-methoxy-3-(phenylmethoxy)-, (17 $\beta$ )- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.



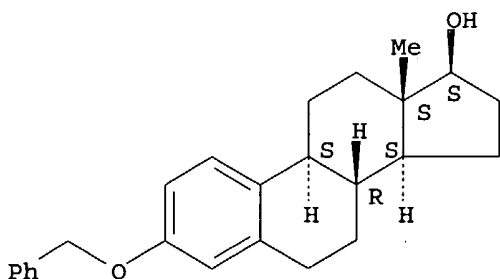
IT **14982-15-1P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and methylation of)

RN 14982-15-1 HCAPLUS

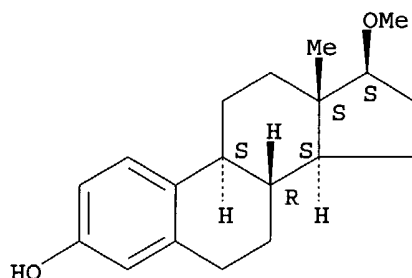
CN Estra-1,3,5(10)-triene-17-ol, 3-(phenylmethoxy)-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 4954-12-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and radioprotective activity of)  
 RN 4954-12-5 HCAPLUS  
 CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX  
 NAME)

Absolute stereochemistry.



L59 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1991:246452 HCAPLUS  
 DN 114:246452  
 ED Entered STN: 28 Jun 1991  
 TI Aluminum trichloride-N,N-dimethylaniline: a new benzyl and allyl ether  
 cleavage reagent  
 AU Akiyama, Takahiko; Hirofuji, Hajimu; Ozaki, Shoichiro  
 CS Fac. Eng., Ehime Univ., Matsuyama, 790, Japan  
 SO Tetrahedron Letters (1991), 32(10), 1321-4  
 CODEN: TELEAY; ISSN: 0040-4039  
 DT Journal  
 LA English  
 CC 21-2 (General Organic Chemistry)  
 OS CASREACT 114:246452  
 AB Benzyl and allyl ethers were cleaved readily on treatment with AlCl<sub>3</sub> and  
 N,N-dimethylaniline to give parent alcs. in high yields. Comparisons of  
 N,N-dimethylaniline and anisole are also described.  
 ST ether allyl benzyl cleavage; aluminum chloride dimethylaniline ether  
 cleavage  
 IT Bond cleavage  
 (of benzyl and allyl ethers, by aluminum trichloride-dimethylaniline)  
 IT Ethers, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (allyl, ether cleavage of, by aluminum trichloride-dimethylaniline)  
 IT Ethers, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (benzyl, ether cleavage of, by aluminum trichloride-dimethylaniline)  
 IT 121-69-7, N,N-Dimethylaniline, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (ether cleavage by aluminum trichloride and, of benzyl and allyl  
 ethers)  
 IT 7446-70-0, Aluminum trichloride, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (ether cleavage by dimethylaniline and, of benzyl and allyl ethers)  
 IT 6793-92-6, Benzyl p-bromophenyl ether 7278-60-6 64740-44-9  
 69455-04-5 70770-06-8, Benzyl 3-phenylpropyl ether 75364-26-0  
 93981-51-2 96124-85-5 101747-16-4 104330-36-1 133992-66-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (ether cleavage of, by aluminum trichloride-dimethylaniline)  
 IT 50-28-2P, Estra-1,3,5(10)-triene-3,17-diol (17 $\beta$ )-, preparation  
 57-88-5P, Cholest-5-en-3-ol (3 $\beta$ )-, preparation 106-41-2P,

p-Bromophenol 122-97-4P, 3-Phenylpropanol 3360-41-6P, 4-Phenylbutanol  
 6946-99-2P 17608-41-2P 24536-40-1P **55561-42-7P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, by ether cleavage)

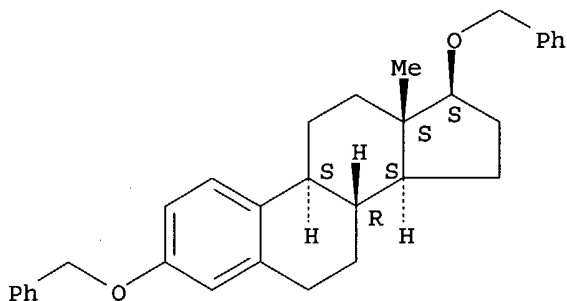
IT **69455-04-5**

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (ether cleavage of, by aluminum trichloride-dimethylaniline)

RN 69455-04-5 HCAPLUS

CN Estradiol-1,3,5(10)-triene, 3,17-bis(phenylmethoxy)-, (17 $\beta$ )- (9CI) (CA  
 INDEX NAME)

Absolute stereochemistry.



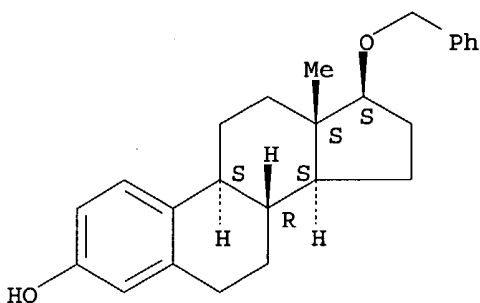
IT **55561-42-7P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, by ether cleavage)

RN 55561-42-7 HCAPLUS

CN Estradiol-1,3,5(10)-trien-3-ol, 17-(phenylmethoxy)-, (17 $\beta$ )- (9CI) (CA  
 INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1990:429367 HCAPLUS

DN 113:29367

ED Entered STN: 21 Jul 1990

TI HPLC determination of steroidal impurities in mestranol and  
 ethynylestradiol

AU Levchenko, N. K.; Osokin, D. M.; Torgov, I. V.; Tuguntaev, G. I.;  
 Sokolova, T. M.; Arzamastsev, A. P.

CS Inst. Bioorg. Khim. im. Shemyakina, Moscow, USSR

SO Khimiko-Farmatsevticheskii Zhurnal (1990), 24(3), 84-6

CODEN: KHFZAN; ISSN: 0023-1134

DT Journal

LA Russian

CC 64-2 (Pharmaceutical Analysis)

AB After TLC separation on a Silufol UV254 plate and identification by using 10% phosphormolybdenic acid in EtOH, steroidal microimpurities were determined in ethynylestradiol and mestranol by HPLC using different columns, mobile phases comprising EtOAc-CHCl<sub>3</sub>, MeHO-CHCl<sub>3</sub>, and CHCl<sub>3</sub>-petroleum ether, and UV spectrophotometric detection at 254 nm. The method is suitable for the quality control of these drugs.

ST ethynylestradiol mestranol impurity detn HPLC; chromatog lig  
ethynylestradiol mestranol impurity; steroid impurity ethynylestradiol mestranol HPLC

IT Steroids, analysis  
RL: ANT (Analyte); ANST (Analytical study)  
(determination of, as impurities in ethynylestradiol and mestranol, by HPLC)

IT Pharmaceutical analysis  
(steroidal impurities determination in ethynylestradiol and mestranol by HPLC in)

IT Chromatography, column and liquid  
(high-performance, steroidal impurities determination in ethynylestradiol and mestranol by)

IT 50-28-2, Estradiol, analysis 53-16-7, Estrone, analysis  
1035-77-4, 3-Methylestradiol 1624-62-0, 3-Methylestrone  
RL: ANT (Analyte); ANST (Analytical study)  
(determination of, as impurity in ethynylestradiol and mestranol, by HPLC)

IT 7627-90-9 33526-46-4, 17 $\beta$ -Methoxyethynylestradiol  
119309-39-6, 17 $\alpha$ -Isobutylestradiol  
RL: ANT (Analyte); ANST (Analytical study)  
(determination of, as impurity in ethynylestradiol, by HPLC)

IT 7548-45-0, 3,17-Dimethoxyethynylestradiol 7627-94-3  
RL: ANT (Analyte); ANST (Analytical study)  
(determination of, as impurity in mestranol, by HPLC)

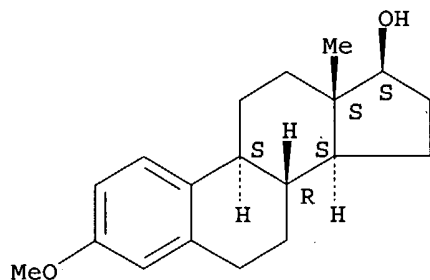
IT 57-63-6 72-33-3, Mestranol  
RL: ANST (Analytical study)  
(steroidal impurities determination in, by HPLC)

IT 1035-77-4, 3-Methylestradiol  
RL: ANT (Analyte); ANST (Analytical study)  
(determination of, as impurity in ethynylestradiol and mestranol, by HPLC)

RN 1035-77-4 HCAPLUS

CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

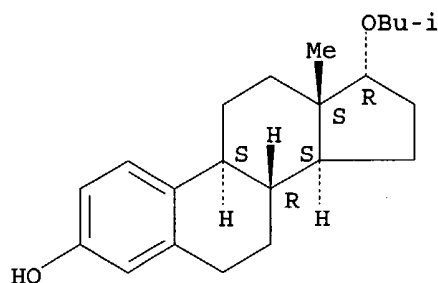


IT 119309-39-6, 17 $\alpha$ -Isobutylestradiol  
RL: ANT (Analyte); ANST (Analytical study)  
(determination of, as impurity in ethynylestradiol, by HPLC)

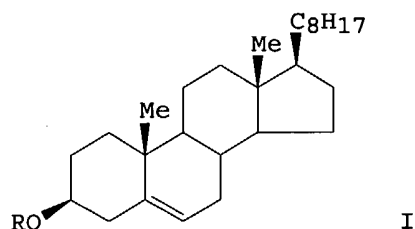
RN 119309-39-6 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-(2-methylpropoxy)-, (17 $\alpha$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1990:158724 HCAPLUS  
 DN 112:158724  
 ED Entered STN: 28 Apr 1990  
 TI Steroids. Part CCCXLIII. Synthesis of 2-propynyl ethers of steroid alcohols  
 AU Pouzar, Vladimir; Schneiderova, Lenka; Drasar, Pavel; Strouf, Oldrich; Havel, Miroslav  
 CS Inst. Org. Chem. Biochem., Slovak Acad. Sci., Prague, 166 10/6, Czech.  
 SO Collection of Czechoslovak Chemical Communications (1989), 54(7), 1888-902  
 CODEN: CCCCAK; ISSN: 0010-0765  
 DT Journal  
 LA English  
 CC 32-7 (Steroids)  
 OS CASREACT 112:158724  
 GI



AB Title ethers were prepared by treating the appropriate hydroxy steroid with CH.tplbond.CCH2Br under conditions of phase-transfer catalysis. Thus, cholesterol (I, R = H) was treated with CH.tplbond.CCH2Br under various phase-transfer conditions to give ether I (R = CH2C.tplbond.CH).  
 ST propynyl ether steroid alc  
 IT Etherification  
 (of hydroxy steroids with propargyl bromide under phase-transfer conditions)  
 IT Steroids, preparation  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (propynyloxy, preparation of, from propargyl bromide under phase-transfer conditions)  
 IT 126003-46-1  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (Oppenauer oxidation of)  
 IT 105644-82-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (detosylation-epimerization of)  
 IT 107-30-2

RL: RCT (Reactant); RACT (Reactant or reagent)  
(etherification by, of androstenediol acetate)

IT 106-96-7, Propargyl bromide  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(etherification by, of hydroxy steroids under phase-transfer conditions)

IT 1639-43-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(etherification of, with chloromethyl Me ether)

IT 53-43-0 57-88-5, Cholesterol, reactions 145-13-1 66168-96-5  
88128-34-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(etherification of, with propargyl bromide under phase-transfer conditions)

IT 58-22-0  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(etherification of,, with propargyl bromide under phase-transfer conditions)

IT 126003-45-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and Oppenauer oxidation of)

IT 126003-31-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and deacetylation of)

IT 126003-33-6P 126003-36-9P 126003-39-2P 126003-43-8P 126003-47-2P  
126024-80-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and deblocking of)

IT 41781-86-6P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and etherification of, with propargyl bromide)

IT 5419-51-2P 126003-32-5P 126003-38-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and etherification of, with propargyl bromide under phase-transfer conditions)

IT 4975-52-4P 18000-76-5P 126003-29-0P 126003-30-3P 126003-34-7P  
126003-35-8P 126003-37-0P 126003-40-5P 126003-41-6P 126003-42-7P  
**126003-44-9P** 126003-48-3P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

IT 110-87-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(O-protection by, of hydroxysteroids)

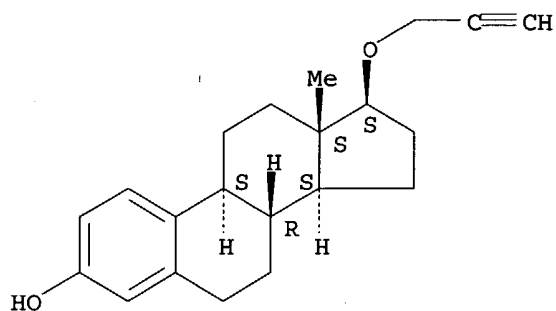
IT 53-16-7, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(O-protection of, with dihydropyran)

IT **126003-44-9P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 126003-44-9 HCAPLUS

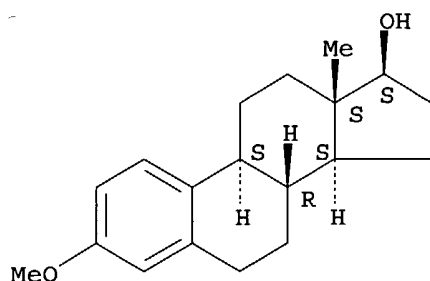
CN Estr-1,3,5(10)-trien-3-ol, 17-(2-propynyloxy)-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1989:121535 HCAPLUS  
 DN 110:121535  
 ED Entered STN: 03 Apr 1989  
 TI High-performance liquid chromatographic analysis of the by-products of the synthesis of ethynylestradiol, mestranol, 17 $\alpha$ -hydroxyprogesterone caproate and 17 $\alpha$ -hydroxy-6-dehydroprogesterone acetate  
 AU Levchenko, N. K.; Osokin, D. M.; Torgov, I. V.; Arzamastsev, A. P.; Sokolova, T. M.; Tuguntaev, G. I.  
 CS M. M. Shemyakin Inst. Bioorg. Chem., Moscow, 117871, USSR  
 SO Journal of Chromatography (1988), 456(2), 427-30  
 CODEN: JOCRAM; ISSN: 0021-9673  
 DT Journal  
 LA English  
 CC 64-3 (Pharmaceutical Analysis)  
 AB Impurities in the samples and mother liquors of title compds. were separated by preparative HPLC on a Prep Pak silica column with a refractometric detector. The compds. were identified by spectral methods and determined by anal. HPLC and TLC. Some of the impurities were estrone, estradiol and estrone Me ethers, 17 $\alpha$ -isobutylestradiol.  
 ST ethynylestradiol impurity detn HPLC; mestranol impurity detn HPLC; hydroxyprogesterone caproate impurity detn HPLC; hydroxydehydroprogesterone acetate impurity detn HPLC; progesterone ester impurity detn HPLC; HPLC steroid impurity detn; chromatog steroid impurity detn  
 IT Steroids, analysis  
 RL: ANST (Analytical study)  
 (determination of impurities in, by HPLC)  
 IT Chromatography, column and liquid  
 (high-performance, of impurities in steroidal drugs)  
 IT 50-28-2, Estradiol, analysis 53-16-7, Estrone, analysis 1035-77-4, Estradiol 3-methyl ether 1624-62-0, Estrone 3-methyl ether 33526-46-4, Ethynylestradiol 17-methyl ether 119309-39-6, 17 $\alpha$ -Isobutylestradiol 119309-40-9, 16-Methoxyethynylestradiol  
 RL: ANT (Analyte); ANST (Analytical study)  
 (determination of, in ethynylestradiol by HPLC)  
 IT 57-63-6, Ethynylestradiol 72-33-3, Mestranol 425-51-4, 17 $\alpha$ -Hydroxy-6-dehydroprogesterone acetate 630-56-8, 17 $\alpha$ -Hydroxyprogesterone caproate  
 RL: AMX (Analytical matrix); ANST (Analytical study)  
 (impurities determination in, by HPLC)  
 IT 1035-77-4, Estradiol 3-methyl ether 119309-39-6, 17 $\alpha$ -Isobutylestradiol  
 RL: ANT (Analyte); ANST (Analytical study)  
 (determination of, in ethynylestradiol by HPLC)  
 RN 1035-77-4 HCAPLUS  
 CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

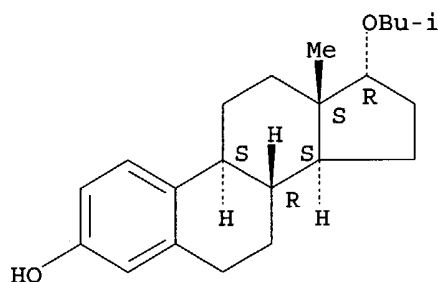
Absolute stereochemistry.



RN 119309-39-6 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-(2-methylpropoxy)-, (17 $\alpha$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1986:62244 HCAPLUS

DN 104:62244

ED Entered STN: 08 Mar 1986

TI Steroid binding to the cytosolic estrogen receptor from rat uterus.  
Influence of the orientation of substituents in the 17-position of the 8 $\beta$ - and 8 $\alpha$ -series

AU Kaspar, Peter; Witzel, Herbert

CS Inst. Biochem., Univ. Muenster, Muenster, D-4400, Fed. Rep. Ger.

SO Journal of Steroid Biochemistry (1985), 23(3), 259-65

CODEN: JSTBBK; ISSN: 0022-4731

DT Journal

LA English

CC 2-2 (Mammalian Hormones)

Section cross-reference(s): 32

AB The exact chemical and sterical requirements in the 17-position of 8 $\beta$ - and 8 $\alpha$ -estrogens for an effective binding to the cytosolic receptor of immature rat uterus were investigated by competition expts. under non-equilibrium conditions. O or N functions with free electron pairs seem to be of essential importance in the 17-position. In contrast to 17 $\alpha$ -methyl-, -vinyl-, or -ethynyl-substituents, a 17 $\alpha$ -Et group strongly disturbs receptor binding. Also, the introduction of a quasi equatorial allene or a 17 $\beta$ -ethynyl group reduces receptor binding. In comparison to the 8 $\beta$ -estrogens, the 8 $\alpha$ -derivs. always showed lower, but still significant receptor binding and similar response to changes of substituents in the 17-position.

ST estrogen receptor steroid binding structure

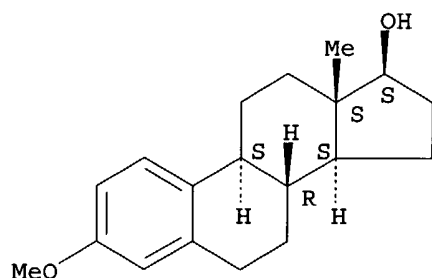
IT Steroids, biological studies

RL: BIOL (Biological study)

- (estrogen receptor binding of, mol. structure in relation to)
- IT Uterus, composition  
(estrogen receptors of, steroids binding by, mol. structure in relation to)
- IT Receptors  
RL: BIOL (Biological study)  
(for estrogen, of uterus, steroids binding by, mol. structure in relation to)
- IT Estrogens  
RL: BIOL (Biological study)  
(receptors for, of uterus, steroids binding by, mol. structure in relation to)
- IT Cytoplasm  
(cytosol, estrogen receptor of, of uterus, steroids binding by, mol. structure in relation to)
- IT Molecular structure-biological activity relationship  
(estrogen receptor-binding, of steroids)
- IT 53-16-7, biological studies 517-06-6, biological studies  
RL: BIOL (Biological study)  
(decomposition and estrogen receptor binding of, mol. structure in relation to)
- IT 1035-77-4 1743-60-8 2553-34-6 20989-33-7 89471-74-9  
89471-79-4 89497-41-6 89576-56-7 99898-94-9 99946-38-0  
RL: PROC (Process)  
(estrogen receptor binding of, mol. structure in relation to)
- IT 50-28-2, biological studies 53-63-4 57-91-0 302-76-1  
517-04-4  
RL: BIOL (Biological study)  
(estrogen receptor of uterus cytosol binding of, mol. structure in relation to)
- IT 99899-00-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and debenzylation of)
- IT 57-63-6P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and dehydration of)
- IT 7628-02-6P 20989-33-7P 99898-92-7P 99898-95-0P 99946-34-6P  
99946-35-7P 99946-36-8P 99946-37-9P 99946-39-1P 100017-39-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and estrogen receptor binding of, mol. structure in relation to)
- IT 57-63-6P 57-91-0P 4717-38-8P 7678-95-7P 15384-74-4P 99946-33-5P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and estrogen receptor of uterus cytosol binding of, mol. structure in relation to)
- IT 99946-40-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and hydrolysis of)
- IT 99898-93-8P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and isomerization of, estrogen receptor binding and mol. structure in relation to)
- IT 99898-99-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reduction of)
- IT 4245-41-4P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, and its reaction with methanesulfonic acid)

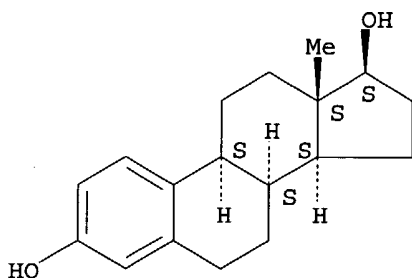
IT 99898-98-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, and its reaction with nitroperbenzoic acid)  
 IT 99898-97-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, and reaction with potassium acetate and methanesulfonic  
 acid and hydrolysis of)  
 IT 5982-51-4  
 RL: BIOL (Biological study)  
 (reduction and estrogen receptor binding of, mol. structure in relation to)  
 IT 1035-77-4  
 RL: PROC (Process)  
 (estrogen receptor binding of, mol. structure in relation to)  
 RN 1035-77-4 HCAPLUS  
 CN Estradiol, 17-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX  
 NAME)

Absolute stereochemistry.



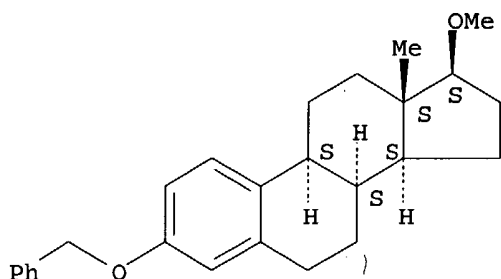
IT 517-04-4  
 RL: BIOL (Biological study)  
 (estrogen receptor of uterus cytosol binding of, mol. structure in  
 relation to)  
 RN 517-04-4 HCAPLUS  
 CN Estradiol, 17-hydroxy-, (17 $\beta$ )- (9CI) (CA INDEX  
 NAME)

Absolute stereochemistry.



IT 99899-00-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and debenzoylation of)  
 RN 99899-00-0 HCAPLUS  
 CN Estradiol, 17-methoxy-3-(phenylmethoxy)-, (17 $\beta$ )- (9CI) (CA INDEX  
 NAME)

Absolute stereochemistry.



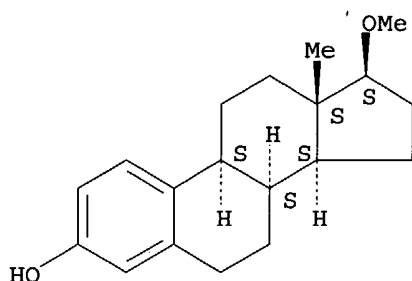
IT 100017-39-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and estrogen receptor binding of, mol. structure in relation to)

RN 100017-39-8 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (8 $\alpha$ ,17 $\beta$ )- (9CI) (CA  
INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1984:96847 HCAPLUS

DN 100:96847

ED Entered STN: 12 May 1984

TI Specificity of an estrogen binding protein in the human vagina compared with that of estrogen receptors in different tissues from different species

AU Bergink, E. W.; Kloosterboer, H. J.; Van der Velden, W. H. M.; Van der Vies, J.; De Winter, M. S.

CS Sci. Dev. Group, Organon Int. B.V., Oss, Neth.

SO Progress in Cancer Research and Therapy (1983), 25(Steroids Endometrial Cancer), 77-84

CODEN: PCRTDK; ISSN: 0145-3726

DT Journal

LA English

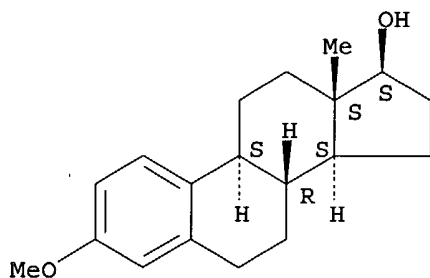
CC 2-2 (Mammalian Hormones)

AB Estrogen-binding proteins from the myometrium, pituitary, thymus, and vagina of the rabbit; myometrium, endometrium, and vagina of the rat; and myometrium, breast tumor tissue, and MCF-7 cells of the human all displayed similar specificities with characteristics of an estrogen receptor. However, the specificity of the estrogen-binding protein in the human vagina was different from that of the human estrogen receptor; the estrogen-binding protein displayed high affinities for 17 $\beta$ -estradiol [50-28-2], 17 $\alpha$ -estradiol [57-91-0], and estriol [50-27-1], but a relatively low affinity for stilbestrol [56-53-1]. Structural requirements of estrogens for binding to the estrogen receptor in the rabbit myometrium were determined and discussed.

ST estrogen binding protein vagina; receptor estrogen structure activity

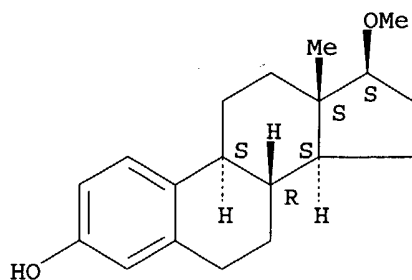
- IT Receptors  
 RL: BIOL (Biological study)  
 (estrogen binding by, in human and laboratory animal, structure in relation to)
- IT Neoplasm, composition  
 (estrogen receptor of, of mammary gland of human, specificity of)
- IT Pituitary gland  
 Thymus gland  
 (estrogen receptor of, specificity of)
- IT Vagina  
 (estrogen-binding protein of, of human and laboratory animal, specificity of)
- IT Estrogens  
 RL: PROC (Process)  
 (receptor binding of, in human and laboratory animal, structure in relation to)
- IT Molecular structure-biological activity relationship  
 (estrogen receptor-binding, of estrogens, in human and laboratory animal)
- IT Proteins  
 RL: BIOL (Biological study)  
 (estrogen-binding, of vagina, of human, specificity of)
- IT Uterus, composition  
 (myometrium, estrogen receptor of, of human and laboratory animal)
- IT Mammary gland  
 (neoplasm, estrogen receptor of, of human, specificity of)
- IT 50-27-1 50-28-2, biological studies 52-76-6 52-77-7 53-63-4  
 56-53-1 57-63-6 57-91-0 72-33-3 302-76-1 362-05-0 570-30-9  
 1035-77-4 1162-60-3 1229-24-9 1231-93-2 1464-61-5  
 1818-12-8 2529-54-6 2529-64-8 3398-11-6 3597-38-4 3704-15-2  
 4954-12-5 5444-22-4 6544-69-0 10448-97-2  
 10540-29-1 13570-81-5 13655-95-3 23637-93-6 34816-55-2  
 54502-78-2 54567-02-1 58212-59-2 58212-69-4 59077-04-2  
 66463-44-3 88899-71-2 88899-72-3 88899-73-4 88899-74-5  
 88899-75-6 88899-76-7 88930-00-1 88930-01-2  
 RL: PROC (Process)  
 (estrogen receptor binding of, in human and laboratory animals, structure in relation to)
- IT 1035-77-4 4954-12-5 6544-69-0  
 RL: PROC (Process)  
 (estrogen receptor binding of, in human and laboratory animals, structure in relation to)
- RN 1035-77-4 HCAPLUS  
 CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



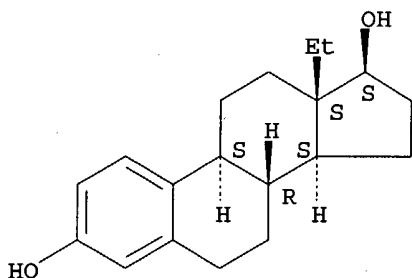
- RN 4954-12-5 HCAPLUS  
 CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

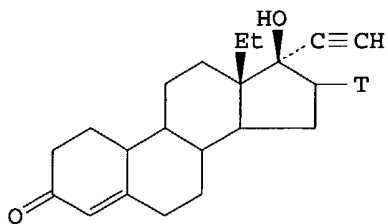


RN 6544-69-0 HCAPLUS  
 CN Gona-1,3,5(10)-triene-3,17-diol, 13-ethyl-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1984:22887 HCAPLUS  
 DN 100:22887  
 ED Entered STN: 12 May 1984  
 TI Tritium NMR spectroscopy of steroids  
 AU Funke, Carel W.; Kasperen, Frans M.; Wallaart, Jan; Wagenaars, Gerard N.  
 CS Sci. Dev. Group, Organon, Oss, 5340 BH, Neth.  
 SO Journal of Labelled Compounds and Radiopharmaceuticals (1983),  
 20(7), 843-53  
 CODEN: JLCRD4; ISSN: 0362-4803  
 DT Journal  
 LA English  
 CC 32-5 (Steroids)  
 Section cross-reference(s): 22  
 GI



I

AB Seven tritiated pregnane-type steroids, e.g. I, were prepared and their T NMR spectra were studied; these spectra gave quant. information on the T

distribution in these compds.

ST tritium NMR steroid

IT Nuclear magnetic resonance  
(of tritium, in pregnanes)

IT Steroids, properties  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(hydroxy, tritium-labeled, preparation and NMR of)

IT **85391-72-6**  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(exchange reaction of, with tritium)

IT **88247-77-2P** 88247-78-3P 88247-79-4P 88247-80-7P  
88255-64-5P 88255-65-6P 88255-66-7P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and NMR of)

IT 73991-16-9 88247-81-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reduction-tritiation of)

IT 54024-21-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(tritiation and ethynylation of)

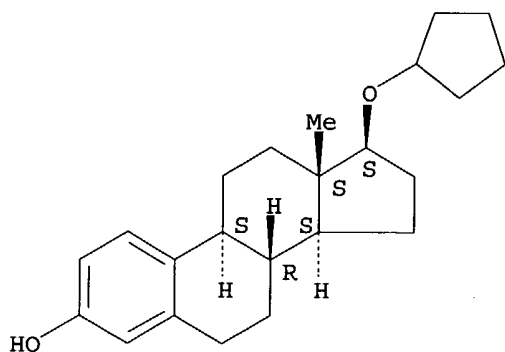
IT 87863-63-6 88247-82-9 88247-84-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(tritiation, ethynylation, and hydrolysis of)

IT **85391-72-6**  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(exchange reaction of, with tritium)

RN 85391-72-6 HCAPLUS

CN Estr-1,3,5(10)-trien-3-ol, 17-(cyclopentyloxy)-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

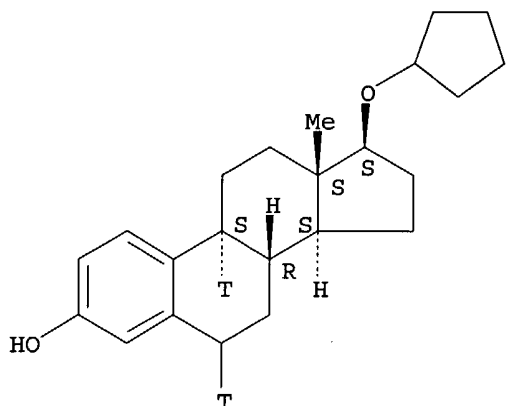


IT **88247-77-2P**  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and NMR of)

RN 88247-77-2 HCAPLUS

CN Estr-1,3,5(10)-trien-6,9-t2-3-ol, 17-(cyclopentyloxy)-, (17 $\beta$ )- (9CI)  
(CA INDEX NAME)

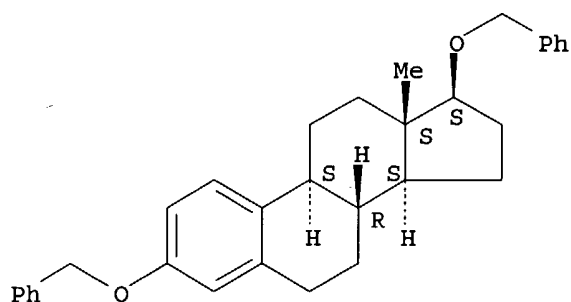
Absolute stereochemistry.



- L59 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1979:202998 HCAPLUS  
 DN 90:202998  
 ED Entered STN: 12 May 1984  
 TI Hard acid and soft nucleophile system. New efficient method for removal of benzyl protecting group  
 AU Fuji, Kaoru; Ichikawa, Kohei; Node, Manabu; Fujita, Eiichi  
 CS Inst. Chem. Res., Kyoto Univ., Uji, Japan  
 SO Journal of Organic Chemistry (1979), 44(10), 1661-4  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DT Journal  
 LA English  
 CC 21-1 (General Organic Chemistry)  
 Section cross-reference(s): 25, 30, 32  
 AB Aliphatic and aromatic benzyl ethers were cleaved on treatment with a hard acid, F3B.OEt2, and a soft nucleophile, EtSH or HSCH2CH2SH, to give parent alcs. and phenols, resp. Competitive debenzylation expts. showed that the coordination of a hard acid (pulling factor) is more important than the nucleophilic attack of a soft nucleophile to the carbon atom (pushing factor) in this reaction. Thus, benzyl 2-naphthyl ether was treated with F3B.OEt2 and EtSH at room temperature for 0.8 h to give 92% 2-naphthol. Treatment of estradiol dibenzyl ether (I) with F3B.OEt2 and EtSH in CH2Cl2 at room temperature for 3 h gave 26.39% I, 11.7% estradiol 17-monobenzyl ether, 17.5% 3-monobenzyl ether, and 30.1% estradiol.  
 ST debenzylation benzyl ether ethanethiol; boron trifluoride debenzylation benzyl ether; nucleophile hard soft debenzylation; protecting group benzyl cleavage; estradiol benzyl ether debenzylation; naphthol benzyl ether debenzylation  
 IT Steroids, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (benzyloxy, debenzylation of, by hard-soft nucleophile system)  
 IT Debenzylation  
 (of benzyl ethers by hard-soft nucleophile system)  
 IT Protective groups  
 (benzyl, removal of, by hard-soft nucleophile system)  
 IT Terpenes and Terpenoids, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (benzyloxy, debenzylation of, by hard-soft nucleophile system)  
 IT Nucleophiles  
 (hard-soft, debenzylation by, of benzyl ethers)  
 IT 3839-48-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (Grignard reaction of, with (benzyloxy)bromotoluene derivative)

- IT 2973-78-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(benzylation of)
- IT 613-62-7 1145-76-2 2830-53-7 5333-62-0 6793-92-6 69455-01-2  
69455-02-3 69455-03-4 **69455-04-5** 69455-05-6 69455-06-7  
69461-89-8 69461-90-1 69483-57-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(benzylation of, by hard acid and soft nucleophile system)
- IT 834-25-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(competitive debenzylation with bromophenyl benzyl ether, by hard-soft nucleophile system)
- IT 75-08-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(debenzylation by, of aliphatic and aromatic benzyl ethers)
- IT 69455-09-0  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(debenzylation of)
- IT 69455-11-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and Wittig reaction of)
- IT 69455-12-5P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and bioketalization of)
- IT 69455-10-3P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)
- IT 50-28-2P, preparation 80-97-7P 89-83-8P 100-02-7P, preparation  
106-41-2P 135-19-3P, preparation 6627-55-0P 13853-46-8P  
13947-29-0P 69455-07-8P 69455-08-9P 69483-58-5P 69483-59-6P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, by debenzylation of benzyl ether by hard-soft nucleophile system)
- IT **14982-15-1P 55561-42-7P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, by debenzylation of estradioldibenzyl ether with hard-soft nucleophile system)
- IT 100-44-7, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(substitution reaction of, with bromohydroxybenzaldehyde)
- IT **69455-04-5**  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(benzylation of, by hard acid and soft nucleophile system)
- RN 69455-04-5 HCAPLUS
- CN Estradiol, 1,3,5(10)-triene, 3,17-bis(phenylmethoxy)-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 14982-15-1P 55561-42-7P

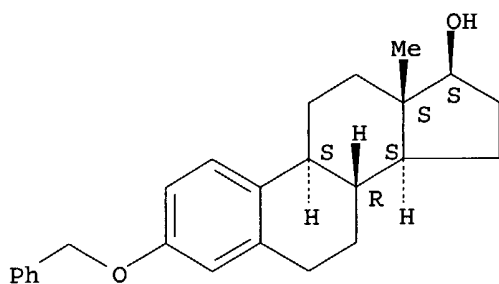
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, by debenzoylation of estradioldibenzyl ether with hard-soft nucleophile system)

RN 14982-15-1 HCAPLUS

CN Estradiol, 3-(phenylmethoxy)-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

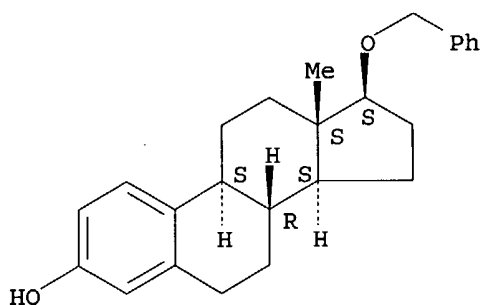
Absolute stereochemistry.



RN 55561-42-7 HCAPLUS

CN Estradiol, 17-(phenylmethoxy)-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1978:402201 HCAPLUS

DN 89:2201

ED Entered STN: 12 May 1984

TI Structural requirements for maximal inhibitory allosteric effect of estrogens and estrogen analogs on glutamate dehydrogenase

AU Pons, Michel; Michel, Francoise; Descomps, Bernard; Crastes de Paulet, Andre

CS Unite Rech. Biochim. Steroides, INSERM, Montpellier, Fr.

SO European Journal of Biochemistry (1978), 84(1), 257-66

CODEN: EJBICAI; ISSN: 0014-2956

DT Journal

LA English

CC 7-3 (Enzymes)

AB The inhibition of glutamate dehydrogenase by estrogens, estrogen analogs, or polyphenylethylene derivs. (.apprx.100 mols., most of them having estrogenic or antiestrogenic activities) was measured. The efficiency of these compds. in inducing allosteric inhibition of the enzyme was compared and correlated to their chemical structure: an aromatic ring A, a free phenolic group in the region of C-3 of the steroid nucleus, and a lipophilic substitution in the region of C-12, C-13, or C-17 were the main structural

features required for maximum efficiency on glutamate dehydrogenase. A tentative model for the relative orientation of the main inhibitor families is proposed. It accounts for most of the kinetic results and can be used as a tool for the selection of affinity labels directed towards the estrogen binding site of glutamate dehydrogenase.

ST glutamate dehydrogenase inhibition estrogen

IT Estrogens

RL: BIOL (Biological study)

(glutamate dehydrogenase inhibition by)

IT Kinetics, enzymic

(of inhibition, of glutamate dehydrogenase)

IT Molecular structure-biological activity relationship

(glutamate dehydrogenase-inhibiting, of estrogens and analogs)

IT 50-27-1 50-28-2, biological studies 53-16-7, biological studies

53-63-4 56-53-1 57-63-6 57-91-0 302-76-1 481-97-0

517-04-4 517-09-9 547-81-9 566-76-7 571-92-6

1035-77-4 1089-78-7 1213-46-3 1667-98-7 1743-60-8

1818-12-8 3398-11-6 3398-12-7 3434-88-6 3597-38-4

3736-22-9 4019-92-5 4245-41-4 4954-12-5 5189-40-2

5444-22-4 5864-38-0 5965-06-0 5976-63-6 5976-73-8

6544-69-0 10161-33-8 10218-59-4 10448-97-2 13010-22-5

13565-53-2 13864-49-8 14418-02-1 14984-42-0 14984-43-1

20796-59-2 21507-14-2 21507-16-4 21583-10-8 22831-81-8

25547-76-6 32295-36-6 33526-45-3 34816-55-2 40128-89-0

41164-28-7 53177-70-1 60973-93-5 61665-15-4 62013-77-8

65928-98-5 65929-00-2 66320-32-9 66422-07-9 66422-09-1

66422-11-5 66422-12-6 66422-14-8 66422-17-1 66422-18-2

66463-40-9 66463-41-0 66463-42-1 66463-43-2 66463-44-3

66463-45-4 66463-46-5 66463-47-6 66463-48-7 66463-49-8

66463-50-1 66495-43-0 66514-24-7 66514-25-8 66514-26-9

66514-27-0 66537-38-0

RL: BIOL (Biological study)

(glutamate dehydrogenase inhibition by)

IT 9029-12-3

RL: PROC (Process)

(inhibition of, by estrogens and analogs)

IT 517-04-4 1035-77-4 3736-22-9 4954-12-5

5864-38-0 6544-69-0 53177-70-1

66514-24-7 66537-38-0

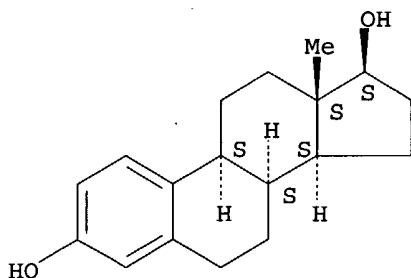
RL: BIOL (Biological study)

(glutamate dehydrogenase inhibition by)

RN 517-04-4 HCAPLUS

CN Estr-1,3,5(10)-triene-3,17-diol, (8 $\alpha$ ,17 $\beta$ )- (9CI) (CA INDEX NAME)

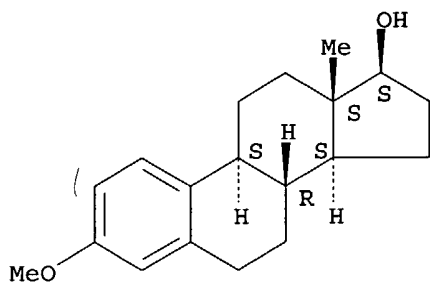
Absolute stereochemistry.



RN 1035-77-4 HCAPLUS

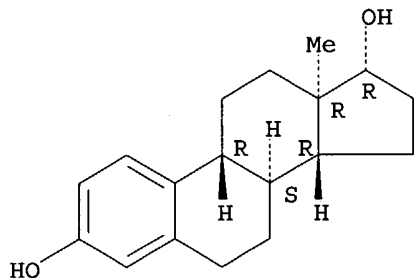
CN Estr-1,3,5(10)-triene-17-ol, 3-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



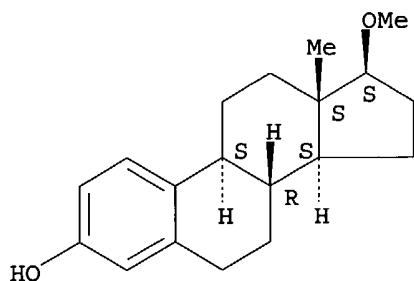
RN 3736-22-9 HCAPLUS  
 CN Estra-1,3,5(10)-triene-3,17-diol, (8 $\alpha$ ,9 $\beta$ ,13 $\alpha$ ,14 $\beta$ ,17 $\alpha$ .)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



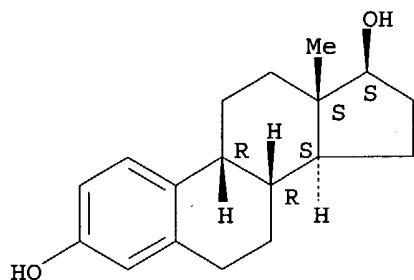
RN 4954-12-5 HCAPLUS  
 CN Estra-1,3,5(10)-triene-3-ol, 17-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



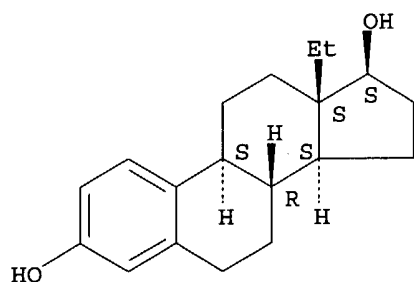
RN 5864-38-0 HCAPLUS  
 CN Estra-1,3,5(10)-triene-3,17-diol, (9 $\beta$ ,17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



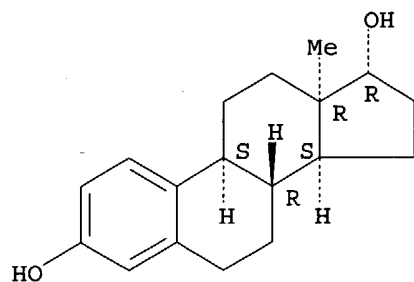
RN 6544-69-0 HCAPLUS  
 CN Gona-1,3,5(10)-triene-3,17-diol, 13-ethyl-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



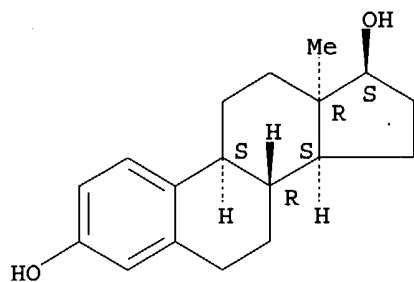
RN 53177-70-1 HCAPLUS  
 CN Estra-1,3,5(10)-triene-3,17-diol, (13 $\alpha$ ,17 $\alpha$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



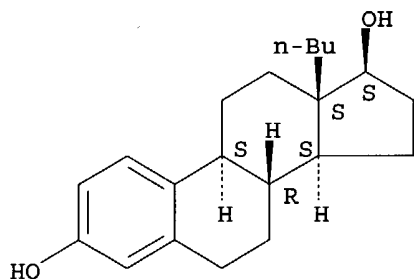
RN 66514-24-7 HCAPLUS  
 CN Estra-1,3,5(10)-triene-3,17-diol, (13 $\alpha$ ,17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



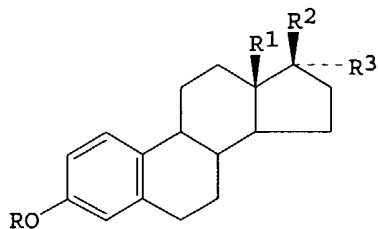
RN 66537-38-0 HCAPLUS  
 CN Gona-1,3,5(10)-triene-3,17-diol, 13-butyl-, (17β)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 16 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1977:90134 HCAPLUS  
 DN 86:90134  
 ED Entered STN: 12 May 1984  
 TI Esterification of phenolic hydroxyl groups in steroids  
 IN Schwarz, Sigfrid; Weber, Gisela  
 PA Ger. Dem. Rep.  
 SO Ger. (East), 5 pp. Addn. to Ger.(East) 114,806.  
 CODEN: GEXXA8  
 DT Patent  
 LA German  
 IC C07C167-28  
 CC 32-3 (Steroids)  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DD 120016	Y	19760520	DD 1975-184239	19750217 <--
PRAI	DD 1975-184239		19750217	<--	
GI					



I

AB Estratrienyl sulfonates I [R = R<sub>4</sub>SO<sub>2</sub>, (R<sub>4</sub> = Me<sub>2</sub>CH, PhCH<sub>2</sub>, Me(CH<sub>2</sub>)<sub>7</sub>, 4-MeC<sub>6</sub>H<sub>4</sub>, cyclopentyl, cyclohexyl); R<sub>1</sub> = H, Me, R<sub>2</sub>R<sub>3</sub> = O, MeON; R<sub>2</sub> = HO, MeO, Me<sub>3</sub>SiO, BuCO<sub>2</sub>, EtCO<sub>2</sub>, PhCH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>, CH<sub>2</sub>:CHCH<sub>2</sub>O; R<sub>2</sub> = H, HC.tplbond.C, ClC.tplbond.C, CH<sub>2</sub>:CH] (20 compds.) were prepared in 76-97% yields by treatment of I (R = H) in H<sub>2</sub>O containing an alkali hydroxide or an alkaline earth hydroxide and a quaternary ammonium salt with R<sub>4</sub>SO<sub>2</sub>Cl. Thus, I (R = R<sub>1</sub> = H, R<sub>2</sub> = OH, R<sub>3</sub> = C.tplbond.CH) in H<sub>2</sub>O-NaOH containing (PhCH<sub>2</sub>)<sub>4</sub>N<sup>+</sup>Cl<sup>-</sup> was treated with Me<sub>2</sub>CHSO<sub>2</sub>Cl to give 80% I (R = Me<sub>2</sub>CHSO<sub>2</sub>, R<sub>1</sub> = H, R<sub>2</sub> = OH, R<sub>3</sub> = C.tplbond.CH).

ST alkanesulfonate estratrienyl; sulfonation norpregnenynol; ethynylestradiol sulfonation; estradiol sulfonation; estrone sulfonation

IT 19-Norsteroids  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (3β-hydroxy-17-oxygenated-1,3,5(10)-unsatd., sulfonates)

IT 28913-23-7P 28913-25-9P 29017-43-4P 29017-44-5P 29017-45-6P  
 32162-69-9P 38022-64-9P 38022-65-0P 42738-04-5P 42738-09-0P  
 42738-11-4P 54983-35-6P 55561-16-5P 55561-21-2P 55561-22-3P  
 55561-24-5P 55561-25-6P 55561-29-0P 55561-31-4P 61872-49-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

IT 1939-99-7 4837-38-1 7795-95-1 10147-37-2 26394-17-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with estradienol)

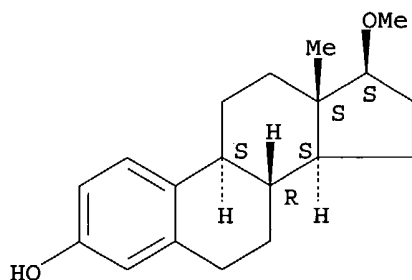
IT 50-28-2, reactions 53-16-7, reactions 57-63-6 3342-64-1 3758-34-7  
 4567-67-3 4954-12-5 7678-95-7 14012-72-7 26443-03-8  
 28416-77-5 33526-46-4 33760-44-0 42737-82-6 55561-41-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (sulfonylation of)

IT 4954-12-5 55561-41-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (sulfonylation of)

RN 4954-12-5 HCAPLUS

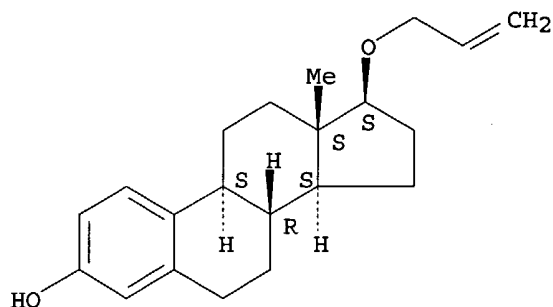
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 55561-41-6 HCAPLUS  
 CN Estra-1,3,5(10)-trien-3-ol, 17-(2-propenyloxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1976:554233 HCAPLUS  
 DN 85:154233  
 ED Entered STN: 12 May 1984  
 TI Study of the specificity of the estradiol-binding system of guinea pig uteri  
 AU Shchedrina, R. N.; Sturchak, S. V.; Bobrova, E. G.; Ishkov, V. L.; Pivnitskii, K. K.; Fanchenko, N. D.  
 CS All-Union Res. Inst. Obstet. Gynecol., Moscow, USSR  
 SO Byulleten Eksperimental'noi Biologii i Meditsiny (1976), 82(8), 989-93  
 CODEN: BEBMAE; ISSN: 0365-9615  
 DT Journal  
 LA Russian  
 CC 2-3 (Hormone Pharmacology)  
 AB The affinities of 49 steroids for the estradiol [50-28-2]-binding system of guinea pig uteri were compared. The presence of free OH groups in positions 3 (phenol) and 17 $\beta$  and reciprocal orientation were required for interaction with the receptor system. An intact steroid skeleton was not necessary. A polar function in ring C inhibited interaction. In addition to estradiol, 17 $\alpha$ -ethynylestradiol [57-63-6], synestrol, and diethylstilbestrol [56-53-1] had high affinities for the estradiol-binding system.  
 ST estradiol receptor interaction estrane deriv  
 IT Uterus, metabolism  
 (estradiol binding by, estrane derivs. in relation to)  
 IT Receptors  
 RL: BIOL (Biological study)  
 (for estradiol, of uterus, estrane derivs. interaction with)  
 IT Estrane, derivs.  
 RL: BIOL (Biological study)  
 (estradiol binding system of uterus interaction with)  
 IT 50-27-1 50-50-0 53-16-7 53-45-2 53-63-4 56-53-1 57-63-6  
 72-33-3 84-16-2 90-15-3 113-38-2 900-83-4 963-75-7 979-32-8  
 1035-77-4 1089-78-7 1125-78-6 1217-09-0 1624-62-0  
 1630-83-7 1852-96-6 2299-08-3 2529-64-8 2639-53-4  
 3736-22-9 6218-29-7 14550-57-3 15833-07-5 19590-55-7  
 32436-64-9 32436-65-0 32436-66-1 34124-99-7 38781-59-8  
 39662-38-9 40481-16-1 54064-57-2 54064-60-7 54064-61-8  
 58395-78-1 60779-03-5 60779-04-6 60779-05-7 60779-06-8  
 60788-62-7 60812-06-8 60827-74-9 60872-64-2  
 RL: BIOL (Biological study)  
 (estradiol binding system of uterus interaction with)  
 IT 50-28-2, biological studies  
 RL: BIOL (Biological study)  
 (uterus binding of)  
 IT 1035-77-4 1852-96-6 3736-22-9  
 38781-59-8

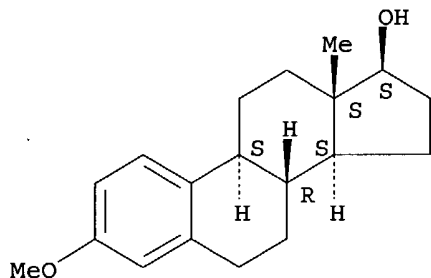
RL: BIOL (Biological study)

(estradiol binding system of uterus interaction with)

RN 1035-77-4 HCAPLUS

CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

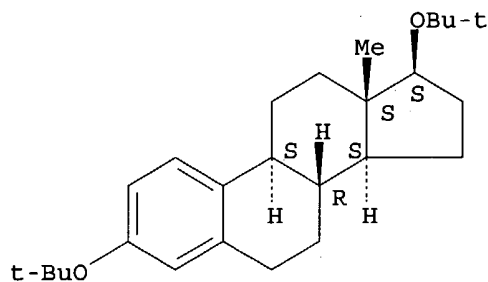
Absolute stereochemistry.



RN 1852-96-6 HCAPLUS

CN Estra-1,3,5(10)-triene, 3,17-bis(1,1-dimethylethoxy)-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

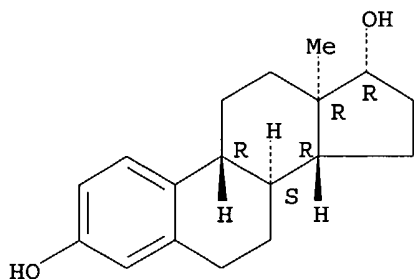
Absolute stereochemistry.



RN 3736-22-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, (8 $\alpha$ ,9 $\beta$ ,13 $\alpha$ ,14 $\beta$ ,17 $\alpha$ .)- (9CI) (CA INDEX NAME)

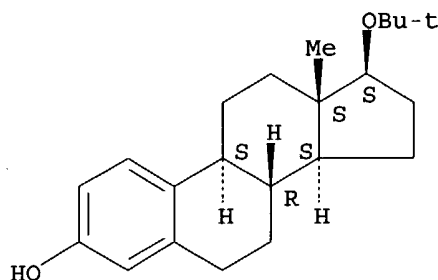
Absolute stereochemistry.



RN 38781-59-8 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-(1,1-dimethylethoxy)-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1975:125520 HCAPLUS  
 DN 82:125520  
 ED Entered STN: 12 May 1984  
 TI Steroids. 15. Sulfonyloxy derivatives of estrogens  
 AU Schwarz, S.; Weber, G.; Schreiber, M.  
 CS Wiss. Lab., VEB Jenapharm, Jena, Ger. Dem. Rep.  
 SO Pharmazie (1975), 30(1), 17-21  
 CODEN: PHARAT; ISSN: 0031-7144  
 DT Journal  
 LA German  
 CC 32-5 (Steroids)  
 GI For diagram(s), see printed CA Issue.  
 AB Estranes I (R = alkyl, cycloalkyl, CH<sub>2</sub>Ph, aminoalkyl; R<sub>1</sub> = C.tplbond.CH, C.tplbond.CCl, CH:CH<sub>2</sub>, Et, H; R<sub>2</sub> = OH, OSiMe<sub>3</sub>, alkoxy, acyloxy; R<sub>1</sub>R<sub>2</sub> = O, NOH, NOSiMe<sub>3</sub>, NOAc, NOME) (66 compds.) were prepared, e.g. by treating the 3-hydroxyestranses with RSO<sub>2</sub>Cl.  
 ST estrane sulfonyloxy; sulfonate estrane; norpregnatrienyl alkanesulfonate; estradiol alkanesulfonate; ethynylestradiol alkanesulfonate  
 IT 19-Norsteroids  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (3-hydroxy-1,3,5(10)-unsatd., sulfonated)  
 IT 41781-86-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (alkylation of)  
 IT 57-63-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (esterification of)  
 IT 1689-02-7 1828-66-6 10147-37-2 10539-95-4 13360-57-1 20588-68-5  
 26394-17-2 35856-62-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (esterification of 17-(trimethylsiloxy)-19-nor-17 $\alpha$ -pregna-1,3,5(10)-trien-20-yn-3-ol by)  
 IT 10147-37-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (esterification of norpregnatrienyndiol)  
 IT 28416-77-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (esterification of, with sulfonyl chlorides)  
 IT 4954-12-5P 55561-41-6P 55561-42-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and esterification of)  
 IT 55561-43-8P 55561-44-9P 55561-45-0P 55561-46-1P 55561-47-2P  
 55561-48-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and etherification of)  
 IT 55561-38-1P 55561-39-2P 55561-40-5P 55561-49-4P 55561-50-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and hydrolysis of)

IT 3381-23-5P 28913-31-7P 28913-32-8P 28913-34-0P 28913-44-2P  
29017-43-4P 29017-44-5P 42738-04-5P 42738-09-0P 42738-11-4P  
52310-88-0P 52310-89-1P 52310-90-4P 54983-32-3P 54983-33-4P  
55561-09-6P 55561-10-9P 55561-11-0P 55561-12-1P 55561-13-2P  
55561-14-3P 55561-16-5P 55612-89-0P 55786-15-7P 55786-17-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and reduction of)

IT 4236-42-4P 28913-23-7P 28913-35-1P 28913-36-2P 54983-34-5P  
54983-35-6P 54983-36-7P 54983-37-8P 54983-38-9P 55561-15-4P  
55561-17-6P 55561-18-7P 55561-19-8P 55561-20-1P 55561-21-2P  
55561-23-4P 55561-24-5P 55561-25-6P 55561-26-7P 55561-27-8P  
55561-28-9P 55561-29-0P 55561-30-3P 55561-31-4P 55561-32-5P  
55561-33-6P 55561-34-7P 55561-35-8P 55561-36-9P 55561-37-0P  
55561-51-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

IT 55561-22-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(preparation, esterification, and etherification of)

IT 4954-12-5P 55561-41-6P 55561-42-7P

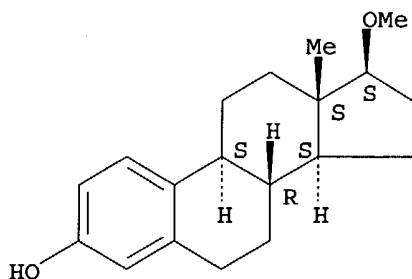
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(preparation and esterification of)

RN 4954-12-5 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX  
NAME)

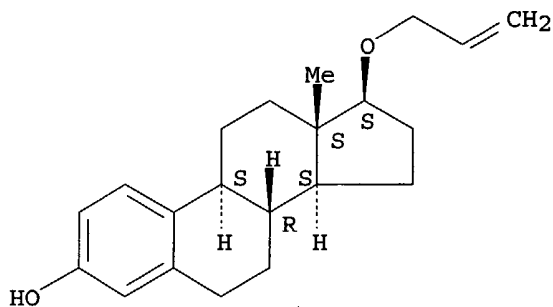
Absolute stereochemistry.



RN 55561-41-6 HCAPLUS

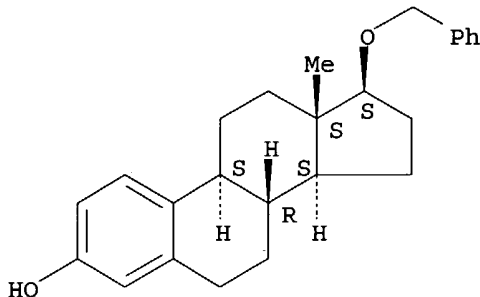
CN Estra-1,3,5(10)-trien-3-ol, 17-(2-propenyloxy)-, (17 $\beta$ )- (9CI) (CA  
INDEX NAME)

Absolute stereochemistry.



RN 55561-42-7 HCAPLUS  
 CN Estradiol 17-(allyloxy) ether, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1974:121187 HCAPLUS  
 DN 80:121187  
 ED Entered STN: 12 May 1984  
 TI Replacing the phenol hydroxy group with hydrogen. Reductive cleavage of alkyl esters of estrogens by lithium in ethers  
 AU Cherkasov, A. N.; Golubovskaya, L. E.; Pivnitskii, K. K.  
 CS Inst. Eksp. Endokrinol. Khim. Gorm., Moscow, USSR  
 SO Zhurnal Organicheskoi Khimii (1974), 10(2), 320-8  
 CODEN: ZORKAE; ISSN: 0514-7492  
 DT Journal  
 LA Russian  
 CC 32-3 (Steroids)  
 GI For diagram(s), see printed CA Issue.  
 AB The estratrienol ether I (R = Me<sub>3</sub>CO) was refluxed in an Ar atmospheric in glyme containing Li to give I (R = HO). Under the same conditions I (R = MeOCH<sub>2</sub>O, tetrahydro-2H-pyran-2-yloxy) yielded I (R = H), and I (R = MeO, Me<sub>2</sub>CHO) gave a mixture of I (R = H, HO). Analogous cleavage products were obtained from estradiol and estrone ethers.  
 ST estratrienol ether cleavage; alkoxyestratriene ether cleavage  
 IT Steroids, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (3-alkoxy-1,3,5(10)-unsatd., reductive cleavage of)  
 IT 50-28-2, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (etherification of)  
 IT 53-16-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (ketalization and etherification of)

IT 38781-61-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

IT 75-26-3 107-30-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with estratrienol)

IT 53-63-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with isopropylbromide)

IT 1852-96-6 3589-91-1 38781-54-3 38781-59-8  
 52509-95-2 52509-96-3 52509-97-4 52610-62-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reductive cleavage of)

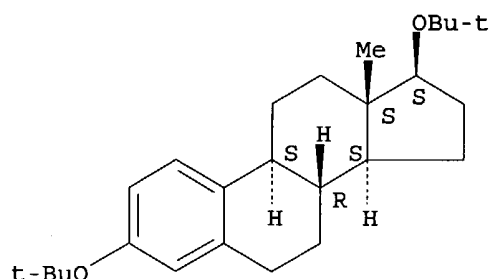
IT 115-11-7, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (with estratrienol)

IT 1852-96-6 38781-59-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reductive cleavage of)

RN 1852-96-6 HCAPLUS

CN Estra-1,3,5(10)-triene, 3,17-bis(1,1-dimethylethoxy)-, (17 $\beta$ )- (9CI)  
 (CA INDEX NAME)

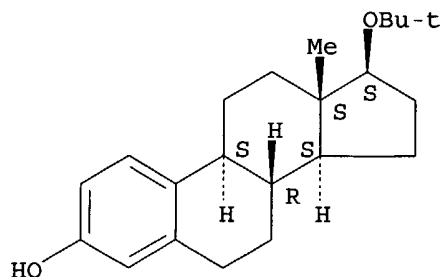
Absolute stereochemistry.



RN 38781-59-8 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-(1,1-dimethylethoxy)-, (17 $\beta$ )- (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1973:533109 HCAPLUS

DN 79:133109

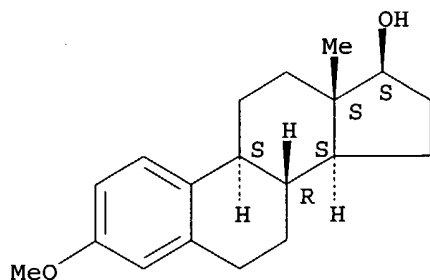
ED Entered STN: 12 May 1984

TI Comparative study of estrogen action

AU Raynaud, Jean P.; Bouton, Marie M.; Gallet-Bourquin, Danielle; Philibert, Daniel; Tournemine, Colette; Azadian-Boulanger, Genevieve

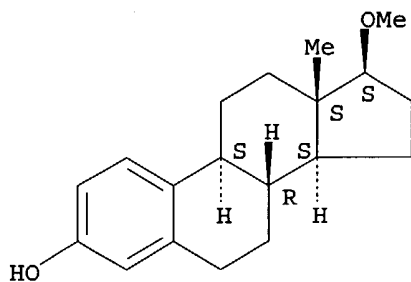
CS Cent. Rech., Roussel-Uclaf, Romainville, Fr.  
 SO Molecular Pharmacology (1973), 9(4), 520-33  
 CODEN: MOPMA3; ISSN: 0026-895X  
 DT Journal  
 LA English  
 CC 2-3 (Hormone Pharmacology)  
 AB The tissue distribution, metabolism, uterine uptake, and plasma and tissue binding of 8estradiol (I) [50-28-2] and 8ethynylestradiol (II) [57-63-6] derivs. were studied in rats in vivo and in vitro, and the results were related to uterotrophic activity. Introduction of a methoxy group in position 11 of II, and especially I, increased uterotrophic activity, whereas methylation of OH groups in positions 3 and 17 decreased it. Uterotropic activity was directly related to binding of the compds. by the 8 S uterine cytosol receptor in vivo. Activity could not be related to binding in vitro. Binding to plasma was not a prerequisite for activity but could modulate it.  
 ST estradiol deriv uterotrophic; ethynylestradiol deriv uterotrophic; uterotrophic estradiol deriv  
 IT Cytoplasm  
 (estradiol derivs. binding by, of uterus, uterotrophic activity of in relation to)  
 IT Blood plasma  
 (estradiol derivs. metabolism by, uterotrophic activity in relation to)  
 IT Uterus, metabolism  
 (of estradiol derivs., uterotrophic activity in relation to)  
 IT Molecular structure-biological activity relationship  
 (uterotropic, of estradiol derivs.)  
 IT 50-28-2, biological studies 57-63-6 72-33-3 1035-77-4  
 4954-12-5 4954-14-7 7548-45-0 21507-14-2  
 21507-16-4 21507-17-5 33526-45-3 33526-46-4 33526-47-5  
 33526-48-6 33713-12-1 34816-55-2  
 RL: BIOL (Biological study)  
 (uterotropic activity of)  
 IT 1035-77-4 4954-12-5 4954-14-7  
 RL: BIOL (Biological study)  
 (uterotropic activity of)  
 RN 1035-77-4 HCAPLUS  
 CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 4954-12-5 HCAPLUS  
 CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

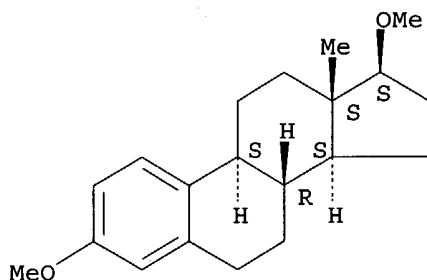
Absolute stereochemistry.



RN 4954-14-7 HCAPLUS

CN Estra-1,3,5(10)-triene, 3,17-dimethoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1973:427594 HCAPLUS

DN 79:27594

ED Entered STN: 12 May 1984

TI Specificity of the estrogen receptor of human uterus

AU Haehnel, Roland; Twaddle, Ella; Ratajczak, Thomas

CS Dep. Obstet. Gynaecol., King Edward Mem. Hosp., Subiaco, Australia

SO Journal of Steroid Biochemistry (1973), 4(1), 21-31

CODEN: JSTBBK; ISSN: 0022-4731

DT Journal

LA English

CC 2-3 (Hormone Pharmacology)

AB The estrogen receptor specificity of the human uterus was determined from the relative abilities of various steroids to compete with 17β-estradiol (I) [50-28-2] for receptor sites in the uterine cytosol fraction. Highest affinity for the receptor required a free phenolic OH group on C3 and an alc. group having the β-configuration at C17, the former being particularly critical. Me groups at C1 or C4 decreased the affinity drastically, whereas the effect of a Me group at C2 was relatively slight. Addnl. O functions in ring D, addnl. substituents on ring A, and unsatn. in ring B decreased the affinity for the receptor, while the presence or absence of the angular Me group at C13 had no influence.

ST steroid uterus estrogen receptor

IT Molecular structure-biological activity relationship  
(estrogen receptor affinity-affecting, of steroids)

IT Uterus

(estrogen receptors of, specificity of)

IT Receptors

RL: BIOL (Biological study)

(for estrogen, of uterus, specificity of)

IT 50-23-7 50-27-1 53-16-7 53-43-0 53-45-2 53-63-4 56-53-1

57-63-6 57-83-0, biological studies 57-91-0 58-22-0 68-96-2  
 145-13-1 434-22-0 474-86-2 481-95-8 481-96-9 481-97-0 517-09-9  
 547-81-9 566-75-6 571-20-0 793-89-5 **1035-77-4** 1090-04-6  
 1150-90-9 1156-92-9 1217-09-0 1228-72-4 1229-33-0 1474-53-9  
 1624-62-0 1806-98-0 1818-12-8 1818-13-9 1818-29-7 1852-50-2  
 1852-53-5 2259-89-4 2479-91-6 2529-64-8 3232-69-7 3233-69-0  
 3434-88-6 3597-38-4 **4954-12-5** 5635-50-7 15093-14-8  
 15270-30-1 20431-33-8 20592-42-1 35577-54-9 35577-55-0  
 42028-17-1 42028-18-2 42028-20-6 42028-21-7

RL: BIOL (Biological study)

(estradiol binding by uterus in response to)

IT 50-28-2, biological studies

RL: BIOL (Biological study)

(receptors for, of uterus, specificity of)

IT **1035-77-4 4954-12-5**

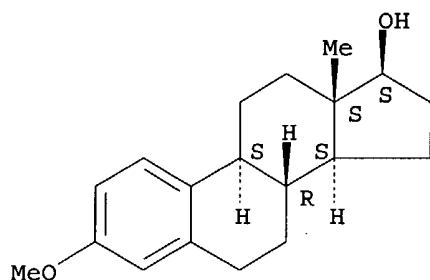
RL: BIOL (Biological study)

(estradiol binding by uterus in response to)

RN 1035-77-4 HCAPLUS

CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

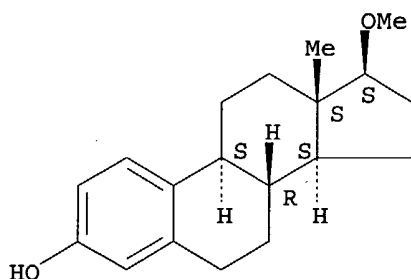
Absolute stereochemistry.



RN 4954-12-5 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1973:106316 HCAPLUS

DN 78:106316

ED Entered STN: 12 May 1984

TI 1,3,5(10)-Estratrien-17 $\beta$ -yl enol ethers and acetals. New classes of orally and parenterally active estrogenic derivatives

AU Gardi, Rinaldo; Vitali, Romano; Falconi, Giovanni; Ercoli, Alberto

CS Warner Vistor Steroid Res. Inst., Casatenovo, Italy

SO Journal of Medicinal Chemistry (1973), 16(2), 123-7

CODEN: JMCMAR; ISSN: 0022-2623

DT Journal  
 LA English  
 CC 2-5 (Hormone Pharmacology)  
 OS CASREACT 78:106316  
 AB A number of labile 17-ethers of estradiol showed uterotrophic activity greater than that of estradiol, and in some cases comparable to that of ethynylestradiol. Especially active orally at 0.3-0.9 nmole/day in mice were cycloalkenyl ethers with 5-9-membered rings, such as 17 $\beta$ -(cyclopent-1-enyloxy)estra-1,3,5(10)-trien-3-ol propionate (I) [13885-28-4], and mixed ketals such as 17 $\beta$ -[(1-methoxycyclopentyl)oxy]estra-1,3,5(10)-trien-3-ol (II) [13885-25-1]. High and long-lasting parenteral uterotrophic activity in rats was shown after single s.c. doses of 0.05  $\mu$ mole of cycloalkenyl ethers with 8-15-membered rings such as 17 $\beta$ -(cyclooct-1-enyloxy)estra-1,3,5(10)-trien-3-ol m-chlorobenzoate [28275-58-3]. The depot activity of these compds. may result from their high lipophilicity and from slow cleavage of the ether linkage to release estradiol. The enol ethers were prepared from the parent 17 $\beta$ -hydroxyestratrienes by acid-catalyzed exchange etherification with alkyl enol ethers or acetals of the appropriate aldehyde or ketone. The acetal and ketal derivs. were prepared by acid-catalyzed addition of the 17 $\beta$ -hydroxy steroid to suitable Me or Et enol ethers.

ST estradiol enol ether estrogen; uterotrophic estradiol enol ether  
 IT Estrogenic hormones  
 RL: BIOL (Biological study)  
 (estratrienyl acetals and enol ethers)

IT Uterus  
 (estratrienyl acetals and enol ethers effect on)

IT Molecular structure-biological activity relationship  
 (estrogenic, of estratrienyl acetals and enol ethers)

IT 53-16-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (acylation of)

IT	3000-64-4P	13885-25-1P	13885-26-2P	13885-27-3P	13885-28-4P
	13885-29-5P	13885-31-9P	13885-32-0P	<b>13885-34-2P</b>	
	13885-35-3P	13885-36-4P	13945-91-0P	13945-92-1P	21513-21-3P
	28151-76-0P	28151-78-2P	28151-79-3P	28151-80-6P	28200-87-5P
	28200-89-7P	28200-91-1P	28200-93-3P	28200-94-4P	28200-96-6P
	28200-97-7P	28200-99-9P	28201-00-5P	28201-01-6P	28201-02-7P
	28201-03-8P	28201-04-9P	28201-05-0P	28231-33-6P	28275-57-2P
	28275-58-3P	28275-59-4P	28275-62-9P	<b>41622-58-6P</b>	
	<b>41622-59-7P</b>	<b>41622-60-0P</b>	41622-64-4P	41622-65-5P	
	<b>41622-66-6P</b>	<b>41622-69-9P</b>	41622-83-7P		
	<b>41622-84-8P</b>	41622-92-8P	41622-93-9P	41622-94-0P	
	41622-95-1P	41622-96-2P	41622-97-3P	41622-98-4P	41622-99-5P
	41623-00-1P	41623-01-2P	41623-02-3P	41623-03-4P	41623-04-5P
	41623-05-6P	41623-06-7P	41623-09-0P	41623-10-3P	41623-11-4P
	41623-12-5P	41623-16-9P	41623-20-5P	41623-21-6P	41680-40-4P
	41787-78-4P				

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and estrogenic activity of)

IT	28151-74-8P	28151-75-9P	28151-77-1P	28200-88-6P	28275-51-6P
	28275-52-7P	28275-53-8P	28275-54-9P	28275-55-0P	28275-56-1P
	41623-22-7P	41623-27-2P	41623-29-4P	41623-30-7P	41623-35-2P
	41623-37-4P	41623-41-0P			

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

IT 502-72-7 931-57-7 41623-39-6  
 RL: BIOL (Biological study)  
 (reaction with estradiol esters)

IT 957-17-5  
 RL: BIOL (Biological study)  
 (reaction with estrones)

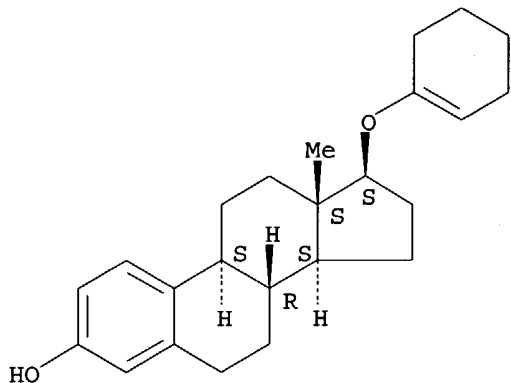
IT 13885-34-2P 41622-58-6P 41622-59-7P  
 41622-60-0P 41622-66-6P 41622-69-9P  
 41622-84-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and estrogenic activity of)

RN 13885-34-2 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-(1-cyclohexen-1-yloxy)-, (17 $\beta$ )- (9CI)  
 (CA INDEX NAME)

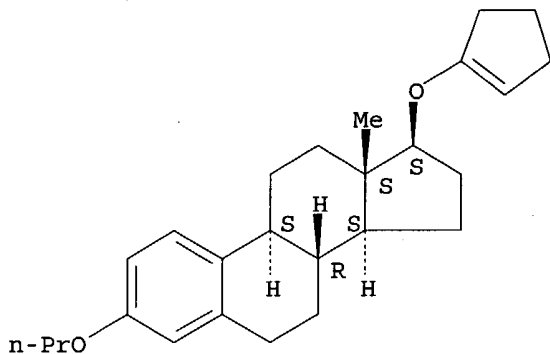
Absolute stereochemistry.



RN 41622-58-6 HCAPLUS

CN Estra-1,3,5(10)-triene, 17-(1-cyclopenten-1-yloxy)-3-propoxy-, (17 $\beta$ )-  
 (9CI) (CA INDEX NAME)

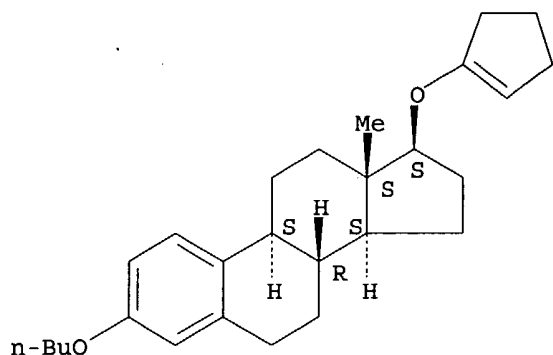
Absolute stereochemistry.



RN 41622-59-7 HCAPLUS

CN Estra-1,3,5(10)-triene, 3-butoxy-17-(1-cyclopenten-1-yloxy)-, (17 $\beta$ )-  
 (9CI) (CA INDEX NAME)

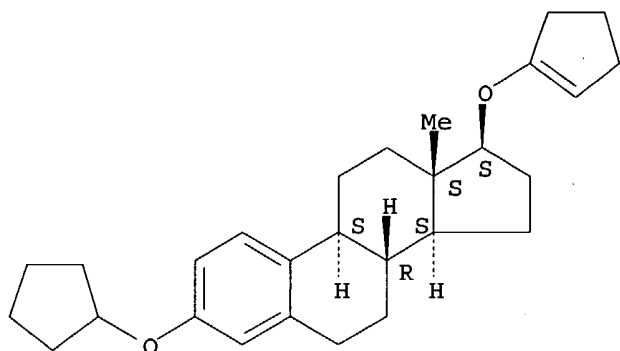
Absolute stereochemistry.



RN 41622-60-0 HCAPLUS

CN Estra-1,3,5(10)-trien-17-(1-cyclopenten-1-yloxy)-3-(cyclopentyloxy)-, (17β)- (9CI) (CA INDEX NAME)

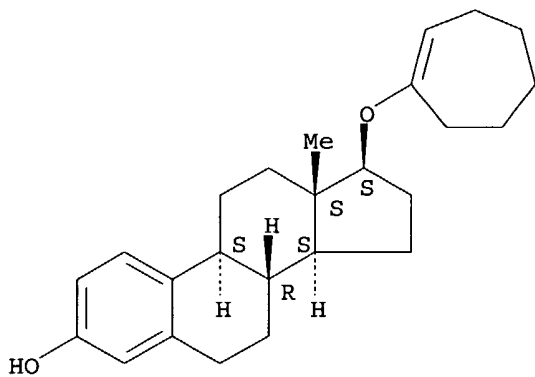
Absolute stereochemistry.



RN 41622-66-6 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-(1-cyclohepten-1-yloxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

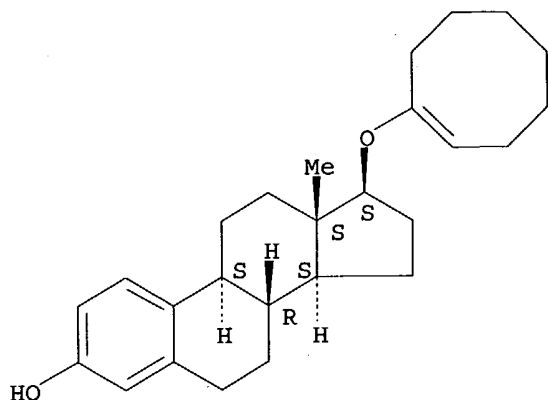


RN 41622-69-9 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-(1-cycloocten-1-yloxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

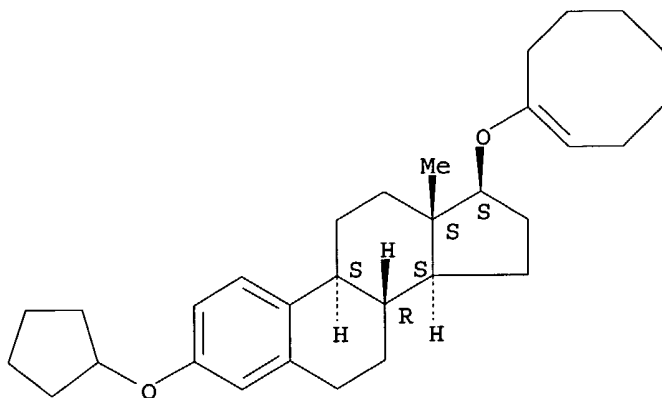


RN 41622-84-8 HCAPLUS

CN Estradiol-1,3,5(10)-triene, 17-(1-cycloocten-1-yloxy)-3-(cyclopentyloxy)-,  
(17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.



L59 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1972:561827 HCAPLUS

DN 77:161827

ED Entered STN: 12 May 1984

TI Degradation of steroids by intestinal bacteria. IV. Aromatization of ring A

AU Goddard, P.; Hill, M. J.

CS Bacterial. Dep., St. Mary's Hosp. Med. Sch., London, UK

SO Biochimica et Biophysica Acta (1972), 280(2), 336-42

CODEN: BBACAQ; ISSN: 0006-3002

DT Journal

LA English

CC 10-2 (Microbial Biochemistry)

AB A strain of Escherichia coli has been shown to produce estradiol from 4-androsten-3,17-dione. From the same substrate a strain of Clostridium paraputrificum produced 17-methoxy-1,3,5(10)-estratriene-3-ol.

ST Escherichia metab androstenedione; Clostridium metab androstenedione; androstenedione bacteria intestine; steroid aromatization gut bacteria

IT Escherichia coli

(estradiol formation from androstendione by)

IT Clostridium paraputrificum

(methoxyestratrienol formation from androstenedione by)

IT 63-05-8  
RL: BIOL (Biological study)  
(aromatization of A of, by intestinal bacteria)

IT 4954-12-5  
RL: FORM (Formation, nonpreparative)  
(formation of, from androstenedione by Clostridium paraputrificum)

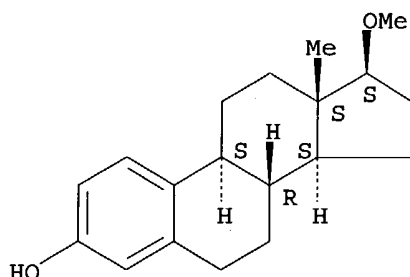
IT 50-28-2, biological studies  
RL: FORM (Formation, nonpreparative)  
(formation of, from androstenedione by Escherichia coli)

IT 4954-12-5  
RL: FORM (Formation, nonpreparative)  
(formation of, from androstenedione by Clostridium paraputrificum)

RN 4954-12-5 HCAPLUS

CN Estradiol, 17-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1972:501990 HCAPLUS

DN 77:101990

ED Entered STN: 12 May 1984

TI New method for the replacement of phenolic hydroxyl group by hydrogen.  
Reduction of alkoxyalkyl ethers of phenols by lithium

AU Cherkasov, A. N.; Pivnitskii, K. K.

CS Inst. Eksp. Endokrinol. Khim. Gorm., Moscow, USSR

SO Zhurnal Organicheskoi Khimii (1972), 8(1), 211-12  
CODEN: ZORKAE; ISSN: 0514-7492

DT Journal

LA Russian

CC 32-3 (Steroids)

AB 3-(Methoxymethoxy)estrane and the tetrahydropyranyl ethers of estranol, estranediol, and estrone ethylene ketal were reduced by finely divided Li in refluxing MeOCH<sub>2</sub>CH<sub>2</sub>OMe to the corresponding 3-H compds. in 76-91% yield. The tert-Bu ethers of estranol and estranediol gave the corresponding phenols in 75-98% yields, resp., under identical conditions.

ST lithium redn steroidal phenol; alkoxyalkoxy steroid redn; dehydroxylation phenol steroidal

IT Steroids, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
((alkoxyalkoxy), dealkoxylation of by lithium)

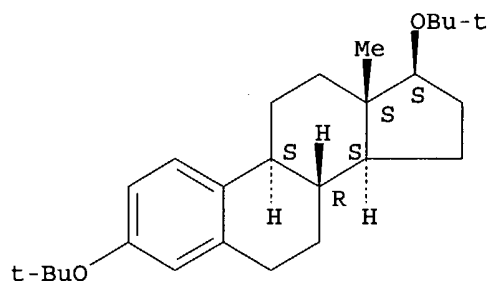
IT Dealkoxylation  
(of (alkoxyalkoxy) steroids, by lithium)

IT 1217-09-0P 38781-61-2P 38781-62-3P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

IT 53-63-4 1852-96-6 3589-91-1 14550-57-3 38781-53-2  
38781-54-3 38781-56-5 38781-57-6 38781-59-8  
RL: RCT (Reactant); RACT (Reactant or reagent)

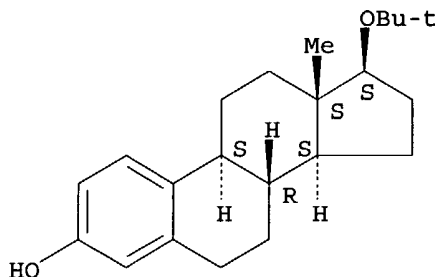
(reaction of, with lithium)  
 IT 7439-93-2, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (with (alkoxyalkoxy)estrane derivs.)  
 IT 1852-96-6 38781-59-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with lithium)  
 RN 1852-96-6 HCAPLUS  
 CN Estra-1,3,5(10)-triene, 3,17-bis(1,1-dimethylethoxy)-, (17 $\beta$ )- (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.



RN 38781-59-8 HCAPLUS  
 CN Estra-1,3,5(10)-trien-3-ol, 17-(1,1-dimethylethoxy)-, (17 $\beta$ )- (9CI)  
 (CA INDEX NAME)

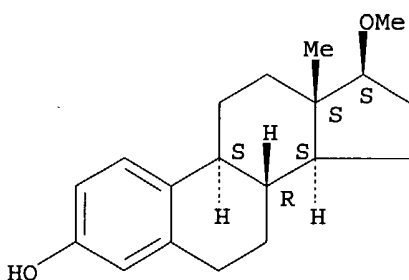
Absolute stereochemistry.



L59 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1972:11880 HCAPLUS  
 DN 76:11880  
 ED Entered STN: 12 May 1984  
 TI Aromatization of androst-4-ene-3,17-dione by human intestinal bacteria  
 AU Goddard, P.; Hill, M. J.  
 CS Dep. Bacteriol., St. Mary's Hosp. Med. Sch., London, UK  
 SO Biochemical Journal (1971), 124(5), 73P  
 CODEN: BIJOAK; ISSN: 0264-6021  
 DT Journal  
 LA English  
 CC 10 (Microbial Biochemistry)  
 AB Clostridium paraputrificum grown anaerobically on broth converted androst-4-ene-3,17-dione to 17 $\beta$ -methoxyestra-1,3,5(10)-trien-3-ol by transfer of the Me group from C-10 to the oxygen on C-17 and aromatization.  
 ST androstenedione metab Clostridium; steroid metab Clostridium; methoxyestratrienol synthesis Clostridium; estratrienol methoxy Clostridium; androgen aromatization bacterial

IT Clostridium paraputrificum  
 (methoxyestratrienol formation by, from androstenedione)  
 IT 63-05-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (aromatization of, by Clostridium paraputrificum)  
 IT 4954-12-5  
 RL: FORM (Formation, nonpreparative)  
 (formation of, from androstenedione by Clostridium paraputrificum)  
 IT 4954-12-5  
 RL: FORM (Formation, nonpreparative)  
 (formation of, from androstenedione by Clostridium paraputrificum)  
 RN 4954-12-5 HCAPLUS  
 CN Estradiol, 1,3,5(10)-trien-3-ol, 17-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1971:459189 HCAPLUS  
 DN 75:59189  
 ED Entered STN: 12 May 1984  
 TI Pharmacodynamic model for studying the mode of action of estrogens using radioactive compounds  
 AU Raynaud, Jean P.; Azadian-Boulanger, Genevieve; Bourquin, Daniele; Philibert, Daniel  
 CS Cent. Rech. Roussel-Uclaf, Romainville, Fr.  
 SO Symp. Progr. Tech. Nucl. Pharmacodyn. (1971), Meeting Date 1970, 39-51. Editor(s): Valette, Guillaume. Publisher: Masson, Paris, Fr. CODEN: 23IDAY  
 DT Conference  
 LA French  
 CC 4 (Hormones and Related Substances)  
 AB Radioactive steroid was injected into prepubertal rats which were then sacrificed. The increased weight of the uterus as well as its incorporation of radioactivity was measured as a function of time, 0 to 70 hr, and anal. was made of estradiol, ethynyl estradiol, and 2 other derivs. The uterus reached a maximum weight at 30-40 hr. The radioactive steroids in the uterus peaked at 1-2 hr and by 10 hr were falling, while estrogen metabolites in the plasma were rising. A math. relation between the weight of the uterus and the concentration of steroid and metabolites is derived.  
 ST estrogen action mode; uterus wt estrogen; plasma metabolite estrogen  
 IT Estrogenic hormones  
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
 (metabolism of, by uterus, mol. structure in relation to)  
 IT Simulation, model  
 (of estrogens metabolism by uterus)  
 IT Uterus, metabolism  
 (of estrogens, model for)  
 IT Molecular structure-biological activity relationships

(uterus-binding, of estrogens)

IT 72-33-3 1035-77-4 4954-12-5 4954-14-7  
 7548-45-0 21507-16-4 21507-17-5 33526-45-3 33526-46-4 33526-47-5  
 33526-48-6 33713-12-1  
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL  
 (Biological study); PROC (Process)  
 (metabolism of, by uterus)

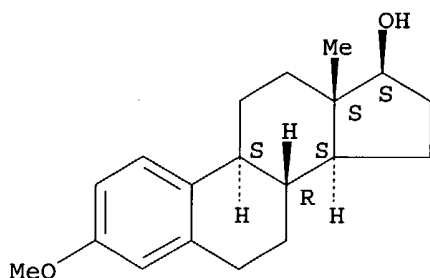
IT 50-28-2, biological studies 57-63-6 21507-14-2 25918-89-2  
 RL: BIOL (Biological study)  
 (uterus binding of, estrogens effect on)

IT 1035-77-4 4954-12-5 4954-14-7  
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL  
 (Biological study); PROC (Process)  
 (metabolism of, by uterus)

RN 1035-77-4 HCAPLUS

CN Estradiol, (17 $\beta$ )- (9CI) (CA INDEX NAME)

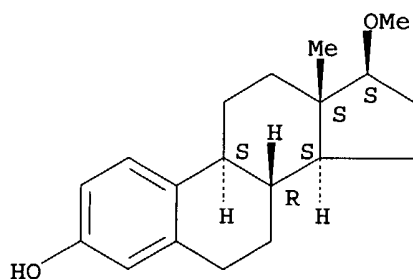
Absolute stereochemistry.



RN 4954-12-5 HCAPLUS

CN Estrone, (17 $\beta$ )- (9CI) (CA INDEX NAME)

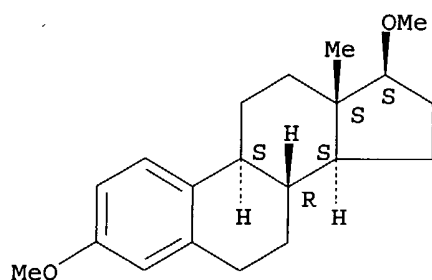
Absolute stereochemistry.



RN 4954-14-7 HCAPLUS

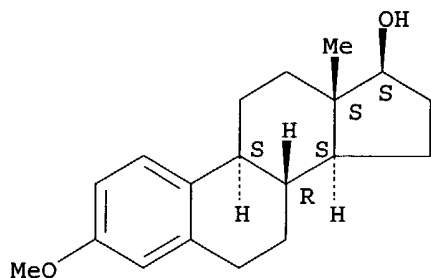
CN Estradiol, 3,17-dimethoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



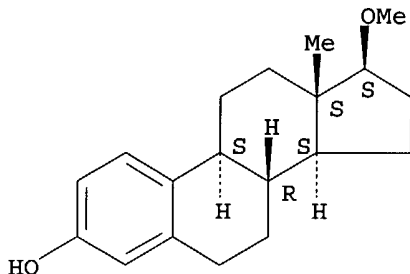
L59 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1970:432065 HCAPLUS  
 DN 73:32065  
 ED Entered STN: 12 May 1984  
 TI Action of natural, synthetic, and semisynthetic estrogens on deciduoma formation in rat uterus  
 AU Yoshino, Akio  
 CS Sch. Med., Jikei Univ., Tokyo, Japan  
 SO Tokyo Joshi Ika Daigaku Zasshi (1969), 84(5), 562-70  
 CODEN: TJIZAF; ISSN: 0040-9022  
 DT Journal  
 LA Japanese  
 CC 4 (Hormones and Related Substances)  
 AB Estrogens (I) priming action was examined with natural synthetic and semisynthetic I on deciduoma formation in rat uterus and metabolism of phospholipid, cholesterol, and nucleic acid in decidual tissue. Female rats, weighing about 160 g, were used at 3 weeks after ovariectomy. Estrone, estradiol, estriol, estrone sulfate, estrone Me ether, estradiol Me ether, estrone benzoate, estradiol benzoate, ethynyl-estradiol, diethylstilbestrol, and hexestrol were used. The natural I were effective primers for the deciduoma formation in rat uterus; synthetic I did not have this action. Natural I had more effect on phospholipid and cholesterol metabolism in rat uterus than synthetic I. Natural and synthetic I showed effects on nucleic acid metabolism.  
 ST estrogens deciduoma uterus; deciduoma uterus estrogens; uterus deciduoma estrogens  
 IT Nucleic acids  
 Phospholipids  
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
 (metabolism of, by uterus, estrogens effect on)  
 IT Uterus, metabolism  
 (of lipids and nucleic acids, estrogens effect on)  
 IT 50-27-1 50-28-2, biological studies 50-50-0 53-16-7, biological studies 56-53-1 57-63-6 481-97-0 1035-77-4 1624-62-0 2393-53-5 4954-12-5 5635-50-7  
 RL: BIOL (Biological study)  
 (lipid and nucleic acid metabolism by uterus in response to)  
 IT 57-88-5, biological studies  
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
 (metabolism of, by uterus, estrogens effect on)  
 IT 1035-77-4 4954-12-5  
 RL: BIOL (Biological study)  
 (lipid and nucleic acid metabolism by uterus in response to)  
 RN 1035-77-4 HCAPLUS  
 CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 4954-12-5 HCAPLUS  
 CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

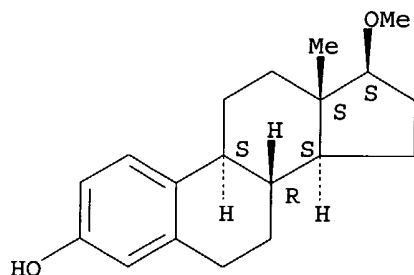


L59 ANSWER 28 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1969:477753 HCAPLUS  
 DN 71:77753  
 ED Entered STN: 12 May 1984  
 TI Mechanism of estrogen action in relation to carcinogenesis  
 AU Jensen, Elwood V.  
 CS Univ. of Chicago, Chicago, IL, USA  
 SO Proceedings of the Canadian Cancer Research Conference (1966),  
 Volume Date 1964, 6, 143-65  
 CODEN: PCCRA4; ISSN: 0068-8436  
 DT Journal  
 LA English  
 CC 4 (Hormones)  
 AB cf. CA 57:6523d. When 3H-labeled estradiol (I) or 17α-methylestradiol (II) was given s.c. in saline to Sprague-Dawley rats, absorption was rapid and the level of radioactivity in the blood and nonresponsive tissues reached a maximum in 15 min., then fell rapidly, while the uterus and vagina continued to incorporate and retain radioactivity. When I or II was given s.c. in sesame oil, the levels in liver and nonresponsive tissues paralleled that in the blood, but in the uterus, vagina, anterior pituitary, and 7,12-dimethylbenz(a)anthracene - induced mammary tumors, there was a progressive uptake and retention. With hexestrol (III), retention in the vagina and uterus was more prolonged. The affinity of the uterus for estriol (IV) was not as striking as for I, but there was some retention in the growth-responsive tissues. The uterus and vagina showed no special affinity for estrone (V). Most of the uterine radioactivity after I administration was in the myometrium. The highest concentration of radioactivity was in the lamina propria with the radioactivity decreasing from the inner to outer myometrium. I was not readily taken up and retained by epithelial cells. After the

administration of 0.1 µg. I, II, or IV, all the radioactivity in the uterus and vagina was in the free steroid fraction after 15 min., 2 hrs., or 6 hrs., resp.; the same was observed in the 2 hr. uteri of III-treated animals. With V, free steroid predominated in the uterus, with some water-soluble radioactivity, but the liver and blood contained radioactivity bound to the alc.-insol. fraction and in the water-soluble form. After administration of I, II, or III, only I, II, or III appeared in the uterus and vagina, while injected IV appeared in the uterus as IV with small amts. of other polar steroids. After V administration, V was present in the uterus after 15 min. but after 2 hrs. V was gone and I was present. Metabolic transformation of I, II, and III occurred in the liver, but I, II, and III evidently stimulate growth in the rat uterus without undergoing metabolic transformation. An early if not initial step in the physiol. action of estrogenic hormones is an association with receptor sites present in the uterus, vagina, and anterior pituitary. Interaction does not involve covalent bonds but is strong enough in vivo to permit the uptake and retention of steroid against a concentration gradient. The initial association of estrogen with receptor sites was inhibited by estrogen antagonists like U-11100 and MER-25 but not actinomycin D or puromycin.

ST  
IT Estrogenic hormones  
RL: BIOL (Biological study)  
(carcinogenesis in relation to)  
IT Neoplasms, metabolism  
(of estrogens in induced mammary)  
IT 50-27-1 50-28-2, biological studies 4954-12-5 5635-50-7  
RL: BIOL (Biological study)  
(in reproductive tract of female after administration)  
IT 4954-12-5  
RL: BIOL (Biological study)  
(in reproductive tract of female after administration)  
RN 4954-12-5 HCAPLUS  
CN Estradiol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 29 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
AN 1969:68634 HCAPLUS  
DN 70:68634  
ED Entered STN: 12 May 1984  
TI 17-Ethers of estradiol  
IN Ercoli, Alberto; Gardi, Rinaldo  
PA Warner-Lambert Pharmaceutical Co.  
SO U.S., 5 pp.  
CODEN: USXXAM  
DT Patent  
LA English  
NCL 424243000  
CC 32 (Steroids)

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3417183	A	19681217	US 1966-546506	19660502 <--
	CH 479568	A	19691015	CH 1966-479568	19660601 <--
	CH 483410	A	19691231	CH 1966-483410	19660601 <--
	DK 118462	B	19700824	DK 1966-2868	19660603 <--
	DK 121437	B	19711018	DK 1969-3171	19690612 <--

PRAI IT 1965-12593 19650604 &lt;--

GI For diagram(s), see printed CA Issue.

AB The title compds. (I) are prepared by treating a 3-ester of estradiol with a functional derivative of a carbonyl compound in the presence of a catalyst. Thus, a solution of 1 g. estradiol 3-propionate (II) in 2 ml. tert-BuOH is treated with 1 ml. cyclopentanone enol methyl ether and 10 mg.

p-MeC<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>H to give the 17-(1-methoxycyclopentyl) (A) ether of II, m. 81-3°, (MeOH-CH<sub>2</sub>Cl<sub>2</sub>), [α]<sub>D</sub><sup>25</sup> 44.5° (c 0.5, dioxane).

Similarly is prepared the A ether of estradiol 3-acetate (III), m.

89-91°, [α]<sub>D</sub><sup>25</sup> 49.5° (c 0.5%, dioxane). A solution of 0.5 g. III in 25 ml. MeOH is refluxed 2 hrs. with 0.1N NaOH, the mixture concentrated, and the residue crystallized from MeOH-CH<sub>2</sub>Cl<sub>2</sub> to give the A

ether of

estradiol, m. 127-9°, [α]<sub>D</sub><sup>25</sup> 50° (c = 0.5, dioxane).

Similarly are prepared the following I [R, R<sub>1</sub>, m.p., and [α]<sub>D</sub><sup>25</sup> (c

0.5, dioxane) given]: EtCO, 1-methoxycyclohexyl, -, 49°; Ac,

1-methoxycyclohexyl, 79-82°, 51.5°; H, 1-methoxycyclohexyl,

108-10°, 53.5°; EtCO, MeOC(Me)Et, 53-7°, 64°;

H, MeOC(Me)Et, 109-13°, 67.5°. A mixture of 3 g. II and 5 ml.

cyclopentanone diethyl acetal is heated 1 hr. at 180-200°,

neutralized with a few drops pyridine, concentrated to dryness in vacuo, and

crystallized from MeOH to give the 17-(cyclopent-1-enyl) ether of II, m.

91-3°, [α]<sub>D</sub><sup>25</sup> 61.5° (c 0.5, dioxane). Similarly are

obtained the following I [R, R<sub>1</sub>, m.p., [α]<sub>D</sub><sup>25</sup> (c 0.5, dioxane)

given]: Ac, cyclopent-1-enyl, 126-8°, 65°; BuCO,

cyclopent-1-enyl, - (oil), 53.5°; H, cyclopent-1-enyl,

73-6°, 66.5°; EtCO, cyclohex-1-enyl, 94-6°,

71°; Ac, cyclohex-1-enyl, 114-16°, 75°; BuCO,

cyclohex-1-enyl, - (oil), 62.5°; H, cyclohex-1-enyl, 87-90°,

75.5°. I possess valuable claudogenic and estrogenic activity,

especially suitable for oral use. It is advisable to stabilize the

pharmaceutical compns. with alkaline substances to prevent acid hydrolysis of the 17-ethers.

ST estradiols estrogenic; estrogenic estradiols

IT 19-Norsteroids

RL: RCT (Reactant); RACT (Reactant or reagent)

(alkoxy)

IT 13885-25-1P 13885-26-2P 13885-27-3P 13885-28-4P 13885-29-5P

13885-30-8P 13885-31-9P 13885-32-0P 13885-33-1P

13885-34-2P 13885-35-3P 13885-36-4P 13885-37-5P

13945-91-0P 13945-92-1P 14258-73-2P 21513-21-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

IT 13885-30-8P 13885-34-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

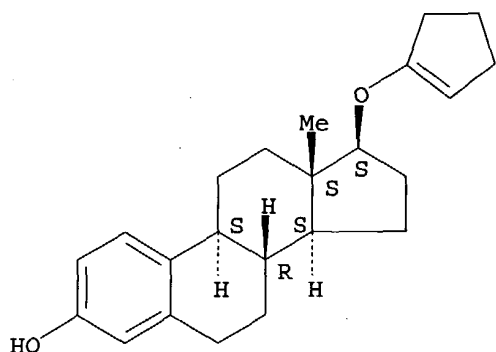
(preparation of)

RN 13885-30-8 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17β-(1-cyclopenten-1-yloxy)- (8CI) (CA

INDEX NAME)

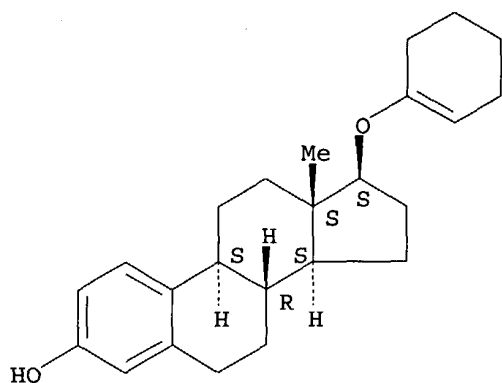
Absolute stereochemistry.



RN 13885-34-2 HCAPLUS

CN Estradiol-1,3,5(10)-trien-3-ol, 17-(1-cyclohexen-1-yloxy)-, (17 $\beta$ )-(9CI)  
(CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1967:95293 HCAPLUS

DN 66:95293

ED Entered STN: 12 May 1984

TI Estradiol ethers

PA Francesco Vismara Societa per Azioni

SO Neth. Appl., 10 pp.

CODEN: NAXXAN

DT Patent

LA Dutch

IC C07C

CC 32 (Steroids)

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	NL 6607527		19661205	NL	<--
	FR 5517			FR	
	GB 1072828			GB	

PRAI IT 19650604 &lt;--

AB Estradiol 3-propionate (I) (1 g.) in 2 cc. tert-BuOH and 1 cc. cyclopentanone enol Me ether treated about 10 min. with 10 mg. p-MeC<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>H yielded the 17-(1-methoxycyclopentyl) ether (II) of I, m. 81-3° (CH<sub>2</sub>Cl<sub>2</sub>-MeOH), [ $\alpha$ ]<sub>D</sub><sup>25</sup> 44.5° (c 0.5, dioxane). Similarly was prepared the 17-(1-methoxycyclopentyl) ether of estradiol

3-acetate (III), m. 89-91°, [ $\alpha$ ]<sub>22D</sub> 49.5° (c 0.5, dioxane). II (0.5 g.) in 25 cc. MeOH refluxed 2 hrs. with 0.1N NaOH gave the 17-(1-methoxycyclopentyl) ether of estradiol (IV), m. 127-9° [(CH<sub>2</sub>Cl)<sub>2</sub>-MeOH]. I (1 g.) in 2 cc. tert-BuOH and 1 cc. cyclohexanone enol Me ether treated with 10 mg. p-MeC<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>H.C<sub>5</sub>H<sub>5</sub>N (V) gave the 17-(1-methoxycyclohexyl) ether (VI) of I. Similarly was prepared 0.95 g. 17-(1-methoxycyclohexyl) ether of III, m. 79-82°, [ $\alpha$ ]<sub>22D</sub> 51.5° (c 0.5, dioxane), from 1 g. III; its hydrolysis with 0.1N KOH gave the 17-(1-methoxycyclohexyl) ether of IV, m. 108-10°, [ $\alpha$ ]<sub>22D</sub> 53.5° (c 0.5, dioxane). I (3 g.) and 5 cc. cyclopentanone dimethyl acetal heated 1 hr. at 180-200° gave the 17-(1-cyclopentenyl) ether (VII) of I, m. 91-3° (MeOH), [ $\alpha$ ]<sub>22D</sub> 61.5° (c 0.5, dioxane). Similarly were prepared the 17-(1-cyclopentenyl) ether of III, m. 126-8°, [ $\alpha$ ]<sub>22D</sub> 65° (c 0.5, dioxane), and the oily 17-(1-cyclopentenyl) ether of estradiol 3-valerate (VIII), [ $\alpha$ ]<sub>22D</sub> 53.5° (c 0.5, dioxane) VII (1.5 g.) in 50 cc. MeOH warmed 2 hrs. with 0.5 g. K<sub>2</sub>CO<sub>3</sub> in 5 cc. H<sub>2</sub>O yielded the 17-(1-cyclopentenyl) ether of IV, m. 73-6°, [ $\alpha$ ]<sub>22D</sub> 66.5° (c 0.5, dioxane). I (2 g.), 3 cc. cyclohexanone dimethyl acetal, 20 mg. V, and 3 cc. HCONMe<sub>2</sub> heated 1 hr. at 180-90° gave the 17-(1-cyclohexenyl) ether (IX) of I, m. 94-6° (CH<sub>2</sub>Cl<sub>2</sub>-MeOH), [ $\alpha$ ]<sub>22D</sub> 71° (c 0.5, dioxane). Similarly were prepared the 17-(1-cyclohexenyl) ether of III, m. 114-16°, [ $\alpha$ ]<sub>22D</sub> 75° (c 0.5, dioxane), and the oily 17-(1-cyclohexenyl) ether of VIII, [ $\alpha$ ]<sub>22D</sub> 62.5° (c 0.5, dioxane). IX (2 g.) hydrolyzed with NaOH-MeOH gave the 17-(1-cyclohexenyl) ether of IV, m. 87-90°, [ $\alpha$ ]<sub>22D</sub> 75.5° (c 0.5, dioxane). EtMeC(OMe)<sub>2</sub> (1 g.), 30 mg. p-MeC<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>H, and 5 cc. tert-BuOH with 1 g. I gave the 17-(1-methoxy-1-methylpropyl) ether of I, m. 64-8°, [ $\alpha$ ]<sub>22D</sub> 62° (c 0.5, dioxane). Similarly was prepared the 17-(1-methoxy-1-methylpropyl) ether of III, m. 53-7°, [ $\alpha$ ]<sub>22D</sub> 64° (c 0.5, dioxane), which hydrolyzed with alkali gave the 17-(1-methoxy-1-methylpropyl) ether of IV, m. 109-13°, [ $\alpha$ ]<sub>22D</sub> 67.5° (c 0.5, dioxane).

ST ESTRADIOL CYCLOPENTYL ETHERS; CYCLOPENTYL ETHERS ESTRADIOL; ESTRADIOL CYCLOHEXYL ETHERS; CYCLOHEXYL ETHERS ESTRADIOL; ESTRADIOL CYCLOPENTENYL ETHERS; CYCLOPENTENYL ETHERS ESTRADIOL; ESTRADIOL CYCLOHEXENYL ETHERS; CYCLOHEXENYL ETHERS ESTRADIOL; ESTRADIOL PROPYL ETHERS

IT Steroids, preparation

RL: PREP (Preparation)

(17-alkoxy)

IT	13885-25-1P	13885-26-2P	13885-27-3P	13885-28-4P	13885-29-5P
	13885-30-8P	13885-31-9P	13885-32-0P	13885-33-1P	
	13885-34-2P	13885-35-3P	13885-36-4P	13885-37-5P	
	13945-91-0P	13945-92-1P	14258-73-2P		

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

IT 13885-30-8P 13885-34-2P

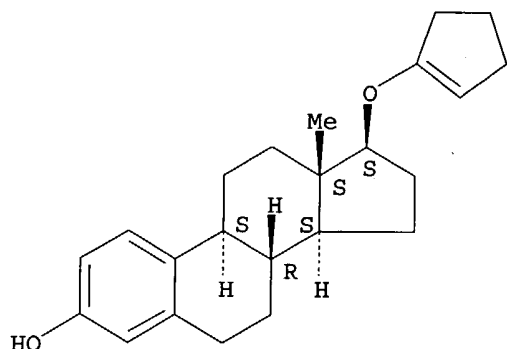
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 13885-30-8 HCAPLUS

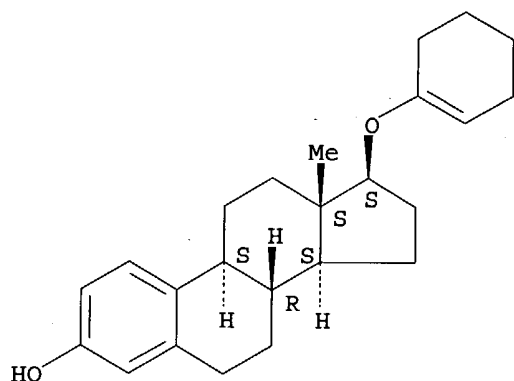
CN Estra-1,3,5(10)-trien-3-ol, 17 $\beta$ -(1-cyclopenten-1-yloxy)- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 13885-34-2 HCAPLUS  
 CN Estra-1,3,5(10)-trien-3-ol, 17-(1-cyclohexen-1-yloxy)-, (17β)- (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1966:44062 HCAPLUS  
 DN 64:44062  
 OREF 64:8257f-g  
 ED Entered STN: 22 Apr 2001  
 TI 17β-Estradiol 17-methyl ether  
 AU Coombs, M. M.; Roderick, H. R.  
 CS Imp. Cancer Res. Fund, Lincoln's Inn Fields, London  
 SO Steroids (1965), 6(6), 841-4  
 CODEN: STEDAM; ISSN: 0039-128X  
 DT Journal  
 LA English  
 CC 42 (Steroids)  
 AB Exptl. results and characterization of various products of  
 17β-estradiol 17-Me ether are presented.  
 IT Dichroism  
 (circular, of 5α-estr-1(10)-en-2-one and 1,10β-dihydro  
 derivative)  
 IT Nuclear magnetic resonance  
 (of 3,17β-dimethoxyestra-1,3,5(10)-triene)  
 IT Estra-1,3,5(10)-triene, 3-(2-benzoyl-4-nitrophenoxy)-2-methoxy-  
 IT 1743-60-8, Estradiol, 17-acetate 4953-96-2, Estra-1,3,5(10)-trien-3-ol,  
 2-methoxy- 4954-12-5, Estra-1,3,5(10)-trien-3-ol,  
 17β-methoxy- 4954-13-6, Estra-1,3,5(10)-trien-3-ol,

17 $\beta$ -methoxy-, benzoate 4954-14-7, Estra-1,3,5(10)-triene,  
 3,17 $\beta$ -dimethoxy- 4954-16-9, Estradiol, 17-acetate,  
 3-p-toluenesulfonate 4954-17-0, Estradiol, 17-acetate, 3-benzoate  
 4967-93-5, Benzophenone, 2-(estra-1,3,5(10)-trien-3-yloxy)-5-nitro-  
 4967-94-6, Estra-1,3,5(10)-triene, 2-methoxy- 4967-96-8,  
 5 $\alpha$ -Estr-1(10)-en-2-one 4968-11-0, Estra-1,3,5(10)-trien-3-ol,  
 17 $\beta$ -methoxy-, acetate 4999-72-8, Benzophenone, 2-[(2-methoxyestra-  
 1,3,5(10)-trien-3-yl)oxy]-5-nitro- 5506-56-9, Benzophenone,  
 2-[(2-hydroxyestra-1,3,5(10)-trien-3-yl)oxy]-5-nitro- 7054-98-0,  
 Estra-2,5(10)-diene, 2-methoxy-

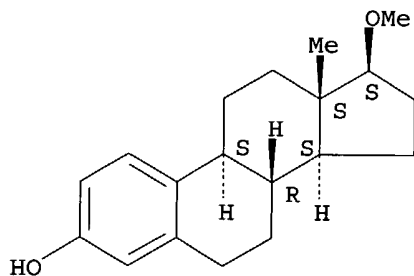
(preparation of)

IT 4954-12-5, Estra-1,3,5(10)-trien-3-ol, 17 $\beta$ -methoxy-  
 4954-14-7, Estra-1,3,5(10)-triene, 3,17 $\beta$ -dimethoxy-  
 (preparation of)

RN 4954-12-5 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX  
 NAME)

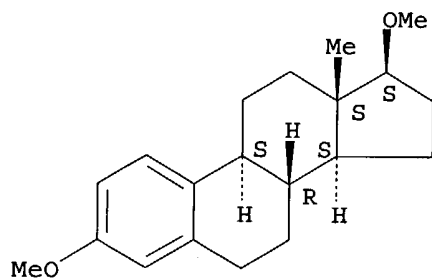
Absolute stereochemistry.



RN 4954-14-7 HCAPLUS

CN Estra-1,3,5(10)-triene, 3,17-dimethoxy-, (17 $\beta$ )- (9CI) (CA INDEX  
 NAME)

Absolute stereochemistry.



L59 ANSWER 32 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1964:493831 HCAPLUS

DN 61:93831

OREF 61:16379g-h

ED Entered STN: 22 Apr 2001

TI Fractionation of estrogen methyl esters and alumina column chromatography  
 (estimation of 16-epiestriol in pregnancy urine)

AU Shida, K.; Kimura, M.; Kanbegawa, A.

CS Med. and Dental Univ. School Med., Tokyo

SO Nippon Naibunpi Gakkai Zasshi (1961), 37(1), 5-9

CODEN: NNGZAZ; ISSN: 0029-0661

DT Journal

LA Unavailable

CC 58 (Hormones)

AB After boiling for 15 min. with 15% concentrated HCl, late pregnancy urine was extracted twice with ether, washed with 5% NaHCO<sub>3</sub> and water, dried with anhydrous

Na<sub>2</sub>SO<sub>4</sub>, and concd, to about 10 ml. in a water bath. The estrogens were extracted with benzene-petr. ether and reextd. with 1.6% NaOH. H<sub>3</sub>BO<sub>3</sub> and dimethyl sulfate were added followed by stirring for 30 min. Following the addition of 30% H<sub>2</sub>O<sub>2</sub> the methylated estrogens were chromatographed on an alumina column 0.5 + 20 cm. prepared by partial filling with petr. ether and the addition of 2.0 g. of Brockmann alumina at 18° under 10-12 mm. Hg. The Me esters of estrone, estradiol, 16-epiestriol, and estriol were eluted with 40% petr. ether in benzene, 1.0% MeOH in benzene, and 3.0% MeOH in benzene, resp. The content of 16-epiestriol reached 11.5% in late pregnancy urine. From Abstract Japan. Med. 1(15), Abstract

Number

6640(1961).

IT Pregnancy

(16-epiestriol in urine in)

IT Urine

(analysis, determination of 16-epiestriol)

IT Estrogenic hormones or principles

(methyl esters, chromatography of)

IT Estra-1,3,5(10)-triene-16 $\alpha$ ,17 $\beta$ -diol, 3-methoxy-

(determination of, in urine in pregnancy)

IT 547-81-9, Estra-1,3,5(10)-triene-3,16 $\beta$ ,17 $\beta$ -triol

1035-77-4, Estra-1,3,5(10)-trien-17 $\beta$ -ol, 3-methoxy-

1624-62-0, Estra-1,3,5(10)-trien-17-one, 3-methoxy-

3434-79-5,

Estra-1,3,5(10)-triene-16 $\beta$ ,17 $\beta$ -diol, 3-methoxy-

4954-12-5, Estra-1,3,5(10)-trien-3-ol, 17 $\beta$ -methoxy-

(determination of, in urine in pregnancy)

IT 1035-77-4, Estra-1,3,5(10)-trien-17 $\beta$ -ol, 3-methoxy-

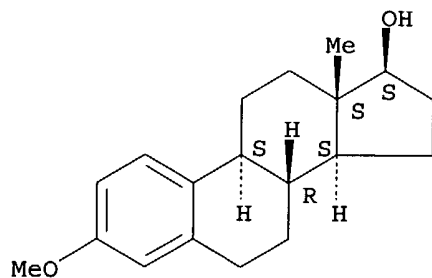
4954-12-5, Estra-1,3,5(10)-trien-3-ol, 17 $\beta$ -methoxy-

(determination of, in urine in pregnancy)

RN 1035-77-4 HCAPLUS

CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

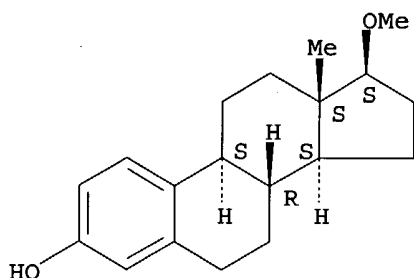
Absolute stereochemistry.



RN 4954-12-5 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 33 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1962:40001 HCAPLUS

DN 56:40001

OREF 56:7630a-d

ED Entered STN: 22 Apr 2001

TI Steroid derivatives. XII. Chromatography of neutral steroids on a thin aluminum oxide layer

AU Hermanek, S.; Schwarz, V.; Cekan, Z.

CS Research Inst. Nat. Drugs, Prague

SO Collection of Czechoslovak Chemical Communications (1961), 26, 1669-79

CODEN: CCCCAK; ISSN: 0010-0765

DT Journal

LA German

CC 55 (Biochemical Methods)

AB cf. CA 55, 27411c; 56, Number 5.-The use of Al<sub>2</sub>O<sub>3</sub> without binder has the advantage of simplicity in preparing a thin layer for chromatography. Alkaline Al<sub>2</sub>O<sub>3</sub> was used with ligroin (b. 30-50°), benzene, ligroinbenzene, and benzene-EtOH mixts. in various proportions. Δ<sup>4</sup>-3-Ketones were detected by lightly spraying with SbCl<sub>3</sub> in CHCl<sub>3</sub>, other Δ<sup>4</sup>-substances with SbCl<sub>3</sub> in CHCl<sub>3</sub> with 10% SOCl<sub>2</sub>. Alkalinity of Al<sub>2</sub>O<sub>3</sub> was without influence on R<sub>f</sub> values and, except for formates, trichloroacetates, and trifluoroacetates, did not degrade the substances during the 10-20 min. of development. Benzene was used as the first solvent for unknown mixts. R<sub>f</sub> values in several solvents are tabulated for some 90 steroids belonging to 3-substituted cholest-5-enes, 17-substituted 3β-acetoxyandrost-5-enes, 3βsubstituted androst-5-en-17-ones, 3β-substituted methyl-7keto-eti-5-enates, 3β-substituted cholest-5-en-7-ones, 17βsubstituted androst-4-en-3-ones, and miscellaneous classes. Chromatographic control of preparation and purity of a substance is exemplified by the separation of pregn-4-ene-17α,21-diol-3,20-dione, its diacetates, 17α,21-diacetoxypregn-5-en3β-ol-20-one, and 17α,21-diacetoxy-3β-formyloxypregn-5en-20-one and accompanying impurities. Adsorptivity of 17β-substituents increased in the following order: COOCH<sub>3</sub>, OBz, CN-COCH<sub>3</sub>, OAc, O, OH; for 3β-substituents of cholest-5-ene the order was: H, Cl, OCH<sub>3</sub>, OAc, OH, and NMe<sub>2</sub>; similarly, cyclohexylamine moved more slowly than cyclohexanol while aniline was much faster than PhOH.

IT Steroids

(separation of, on Al<sub>2</sub>O<sub>3</sub> film)

IT Androst-5-ene-17β-carboxylic acid, 12α-hydroxy-17-methyl-3-oxo-, methyl ester, acetate

Estradiol, propionate

(separation of, on Al<sub>2</sub>O<sub>3</sub> film)

IT Androst-5-ene-17β-carboxylic acid, 12α-hydroxy-17-methyl-3-oxo-, methyl ester

Androst-5-ene-17β-carboxylic acid, 12α-hydroxy-17-methyl-3-oxo-, methyl ester, benzoate

Androst-5-ene-17β-carboxylic acid, 12α-hydroxy-17-methyl-3-oxo-

- , methyl ester, p-toluenesulfonate  
 Cholesterol, nitrobenzoate  
 Pivalic acid, cholesteryl ester  
 (separation on Al2O3 film)
- IT 57-87-4, Ergosterol 83-48-7, Stigmasterol  
 (chromatography of, on Al2O3)
- IT 95908-73-9, Pregn-5-ene-20-carboxylic acid, 3 $\beta$ -hydroxy-, acetate  
 (chromatography on Al2O3)
- IT 142-62-1, Hexanoic acid  
 (esters, separation on Al2O3 film)
- IT 53-16-7, Estrone 53-43-0, Androst-5-en-17-one, 3 $\beta$ -hydroxy-  
 57-83-0, Progesterone 57-88-5, Cholesterol 58-18-4,  
 Androst-4-en-3-one, 17 $\beta$ -hydroxy-17-methyl- 58-22-0, Testosterone  
 63-05-8, Androst-4-ene-3,17-dione 64-85-7, Corticosterone, deoxy-  
 68-96-2, Pregn-4-ene-3,20-dione, 17-hydroxy- 80-75-1,  
 Pregn-4-ene-3,20-dione, 11 $\alpha$ -hydroxy- 145-13-1, Pregn-5-en-20-one,  
 3 $\beta$ -hydroxy- 152-58-9, Pregn-4-ene-3,20-dione, 17,21-dihydroxy-  
 302-23-8, Pregn-4-ene-3,20-dione, 17-hydroxy-, acetate 387-79-1,  
 Pregn-5-en-20-one, 3 $\beta$ ,17-dihydroxy- 434-03-7, 17 $\alpha$ -Pregn-4-en-  
 20-yn-3-one, 17-hydroxy- 512-04-9, Diosgenin 516-15-4,  
 Pregn-4-ene-3,11,20-trione 630-56-8, Pregn-4-ene-3,20-dione,  
 17-hydroxy-, hexanoate 640-87-9, Pregn-4-ene-3,20-dione,  
 17,21-dihydroxy-, 21-acetate 974-23-2, Pregn-5-en-20-one,  
 16 $\alpha$ ,17-epoxy-3 $\beta$ -hydroxy- 1035-77-4,  
 Estra-1,3,5(10)-trien-17 $\beta$ -ol, 3-methoxy- 1061-54-7, Diosgenin,  
 acetate 1235-98-9, 17 $\alpha$ -Pregna-4,20-dien-3-one, 17-hydroxy-  
 3604-60-2, 17 $\alpha$ -Pregn-5-en-20-yne-3 $\beta$ ,17-diol 4139-90-6,  
 Androst-5-ene-17 $\beta$ -carboxylic acid, 3 $\beta$ -hydroxy-, methyl ester,  
 acetate 4954-12-5, Estra-1,3,5(10)-trien-3-ol, 17 $\beta$ -methoxy-  
 6252-45-5, Cholest-5-ene, 3 $\beta$ -[(tetrahydropyran-2-yl)oxy]-  
 14072-39-0, Pregn-5-en-20-one, 16 $\beta$ -bromo-3 $\beta$ ,17-dihydroxy-  
 20272-84-8, Pregna-1,4-dien-20-one, 3 $\beta$ -hydroxy- 20867-15-6,  
 Pregn-5-en-20-one, 3 $\beta$ ,17-dihydroxy-, 3-formate 31823-53-7,  
 Chol-5-enic acid, 3 $\beta$ -hydroxy-, methyl ester, acetate 71205-59-9,  
 Pregna-1,4-dien-20-one, 3 $\beta$ -hydroxy-, acetate 95557-72-5,  
 Pregna-1,4-dien-20-one, 3 $\beta$ -hydroxy-, oxime, acetate 96345-96-9,  
 Cholest-5-ene, 3-chloro- 107158-49-6, Cholest-5-en-3 $\alpha$ -amine,  
 N,N-dimethyl-  
 (separation of, on Al2O3 film)
- IT 50-28-2, Estradiol 56-47-3, Corticosterone, deoxy-, acetate 57-85-2,  
 Testosterone, propionate 126-17-0, Solasodine 521-10-8,  
 Androst-5-ene-3 $\beta$ ,17 $\beta$ -diol, 17-methyl- 521-17-5,  
 Androst-5-ene-3 $\beta$ ,17 $\beta$ -diol 566-28-9, Cholest-5-en-7-one,  
 3 $\beta$ -hydroxy- 570-74-1, Cholest-5-ene 601-57-0, Cholest-4-en-3-one  
 604-32-0, Cholesterol, benzoate 604-35-3, Cholesterol, acetate  
 633-34-1, Androsta-4,6-diene-3,17-dione 809-51-8, Cholest-5-en-7-one,  
 3 $\beta$ -hydroxy-, acetate 853-23-6, Androst-5-en-17-one,  
 3 $\beta$ -hydroxy-, acetate 897-06-3, Androsta-1,4-diene-3,17-dione  
 1045-69-8, Testosterone, acetate 1169-49-9, Testosterone, isobutyrate  
 1174-92-1, Cholest-5-ene, 3 $\beta$ -methoxy- 1175-12-8,  
 Androst-5-ene-3 $\beta$ ,17 $\beta$ -diol, 17-benzoate 1182-65-6, Cholesterol,  
 p-toluenesulfonate 1255-57-8, Testosterone, p-toluenesulfonate  
 1259-22-9, Androst-5-ene-3 $\beta$ ,17 $\beta$ -diol, 3-acetate,  
 17-p-toluenesulfonate 1639-43-6, Androst-5-ene-3 $\beta$ ,17 $\beta$ -diol,  
 3-acetate 1639-44-7, Pregn-5-en-20-one, 3 $\beta$ -hydroxy-, benzoate  
 1778-02-5, Pregn-5-en-20-one, 3 $\beta$ -hydroxy-, acetate 1807-15-4,  
 Pregn-4-ene-3,20-dione, 17,21-dihydroxy-, diacetate 2080-86-6,  
 Androst-5-en-17-one, 3 $\beta$ -hydroxy-, benzoate 2088-71-3, Testosterone,  
 benzoate 2099-26-5, Androst-5-ene-3 $\beta$ ,17 $\beta$ -diol, diacetate  
 4651-48-3, Stigmasterol, acetate 4860-15-5, Solasodine, diacetate  
 5953-63-9, Androst-5-ene-3 $\beta$ ,17 $\beta$ -diol, 3-acetate, 17-benzoate  
 6997-41-7, Cholest-5-en-7-one, 3 $\beta$ -hydroxy-, benzoate 14546-23-7,  
 Cholest-5-en-3 $\beta$ -amine, N,N-dimethyl- 19637-35-5,

Androst-5-en-17-one, 3 $\beta$ -[(tetrahydropyran-2-yl)oxy]- 29163-23-3,  
 Androst-5-en-17-one, 3 $\beta$ -hydroxy-, formate 33854-98-7,  
 Androst-5-ene-3 $\beta$ ,17 $\beta$ -diol, 17-methyl-, 3-acetate 34209-81-9,  
 Pregn-5-en-20-one, 16 $\alpha$ ,17-epoxy-3 $\beta$ -hydroxy-, acetate  
 40768-03-4, Androst-5-ene-3 $\beta$ ,17 $\alpha$ -diol, 3-acetate 17-benzoate  
 41329-03-7, Cholesterol, pivalate 50303-03-2, Androst-5-ene-17 $\beta$ -  
 carbonitrile, 3 $\beta$ -hydroxy-, acetate 96553-92-3, Androst-5-ene-  
 3 $\beta$ ,7 $\beta$ ,17 $\beta$ -triol, 17-methyl-, 3,17-diacetate 96772-72-4,  
 Cholest-5-en-7-one, 3 $\beta$ -hydroxy-, p-toluenesulfonate  
 (separation on Al2O3 film)

IT 1344-28-1, Aluminum oxide

(steroid separation on film of)

IT 1035-77-4, Estra-1,3,5(10)-trien-17 $\beta$ -ol, 3-methoxy-

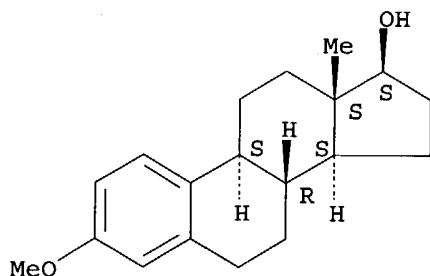
4954-12-5, Estra-1,3,5(10)-trien-3-ol, 17 $\beta$ -methoxy-

(separation of, on Al2O3 film)

RN 1035-77-4 HCAPLUS

CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX  
 NAME)

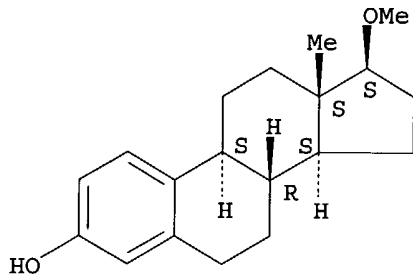
Absolute stereochemistry.



RN 4954-12-5 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX  
 NAME)

Absolute stereochemistry.



=> d his

(FILE 'HOME' ENTERED AT 10:33:36 ON 20 JUL 2004)  
 SET COST OFF

FILE 'HCAPLUS' ENTERED AT 10:34:03 ON 20 JUL 2004

L1 1 S US20020035100/PN OR (US2001-893324# OR WO2001-US41170 OR US20  
 E PROKAI L/AU  
 L2 122 S E3,E4,E7  
 E SIMPKINS J/AU

L3 245 S E3,E5,E7-E9  
SEL RN L1

FILE 'REGISTRY' ENTERED AT 10:35:20 ON 20 JUL 2004

L4 18 S E1-E18  
L5 16 S L4 AND C5-C6-C6-C6/ES  
L6 9 S L5 AND 4/NR  
L7 7 S L5 NOT L6  
L8 STR  
L9 STR L8  
L10 50 S L9  
L11 13381 S L9 FUL  
SAV TEMP L11 QAZI893/A  
L12 STR L9  
L13 22 S L12 CSS SAM SUB=L11  
L14 434 S L12 CSS FUL SUB=L11  
SAV L14 QAZI893A/A  
L15 119 S L14 AND NC>=2  
L16 13 S L15 NOT ((MXS OR PMS OR IDS)/CI OR COMPD OR WITH OR UNSPECIFI  
L17 2 S L16 NOT C18H24O2  
L18 11 S L16 NOT L17  
L19 STR L12  
L20 23 S L19 FUL SUB=L14  
SAV L20 QAZI893B/A  
L21 22 S L20 NOT 13C#  
L22 STR L19  
L23 99 S L22 FUL SUB=L14  
SAV L23 QAZI893C/A  
L24 95 S L23 NOT L15  
L25 87 S L24 NOT (T OR D)/ELS  
L26 12 S L23 NOT L25  
L27 9 S L26 AND C19H26O2  
L28 3 S L26 AND C19H26O2 NOT (T OR D)/ELS  
L29 2 S L28 NOT CYCLODEXTRIN  
L30 STR L19  
L31 58 S L30 FUL SUB=L14  
SAV L31 QAZI893D/A  
L32 57 S L31 NOT (T OR D)/ELS  
L33 169 S L5,L17,L21,L25,L29,L32  
SAV L33 QAZI893E/A  
L34 168 S L33 NOT (T OR D)/ELS  
L35 149 S L14 NOT L15,L34  
L36 89 S L35 NOT (T OR D)/ELS  
L37 46 S L36 NOT IDS/CI  
L38 41 S L37 NOT (11C# OR 13C# OR 14C#)  
L39 39 S L38 NOT PMS/CI

FILE 'HCAPLUS' ENTERED AT 11:19:38 ON 20 JUL 2004

L40 52840 S L34  
L41 1346 S L39  
L42 53115 S L40,L41  
L43 98 S L1-L3 AND L42

FILE 'REGISTRY' ENTERED AT 11:20:19 ON 20 JUL 2004

L44 1 S 50-28-2  
L45 167 S L34 NOT L44  
L46 38 S L39 NOT 57-91-0

FILE 'HCAPLUS' ENTERED AT 11:21:54 ON 20 JUL 2004

L47 605 S L45  
L48 148 S L46  
L49 715 S L47,L48  
L50 9 S L1-L3 AND L49

L51 706 S L49 NOT L50  
L52 654 S L51 AND (PD<=20000627 OR AD<=20000627 OR PRD<=20000627)

FILE 'REGISTRY' ENTERED AT 11:24:14 ON 20 JUL 2004

L53 33 S L45,L46 AND (C26H40O2 OR C24H36O2 OR C22H32O2)  
L54 5 S L20 AND L53  
L55 28 S L53 NOT L54  
L56 18 S L20 NOT L54  
L57 17 S L56 NOT 13C#

FILE 'HCAPLUS' ENTERED AT 11:26:54 ON 20 JUL 2004

L58 41 S L54 OR L57  
L59 33 S L58 AND L52

FILE 'USPATFULL, USPAT2' ENTERED AT 11:27:18 ON 20 JUL 2004

L60 5 S L54 OR L57

FILE 'REGISTRY' ENTERED AT 11:27:37 ON 20 JUL 2004

FILE 'USPATFULL, USPAT2' ENTERED AT 11:29:09 ON 20 JUL 2004

FILE 'HCAPLUS' ENTERED AT 11:29:20 ON 20 JUL 2004

=> => fil reg

FILE 'REGISTRY' ENTERED AT 11:31:00 ON 20 JUL 2004

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 19 JUL 2004 HIGHEST RN 713066-32-1

DICTIONARY FILE UPDATES: 19 JUL 2004 HIGHEST RN 713066-32-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d ide can tot 121

L21 ANSWER 1 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN

RN 623942-19-8 REGISTRY

CN Estr-1,3,5(10)-trien-3-ol, 17-ethoxy-, (8 $\alpha$ ,17 $\beta$ )-(±)-(9CI)  
(CA INDEX NAME)

FS STEREOSEARCH

MF C20 H28 O2

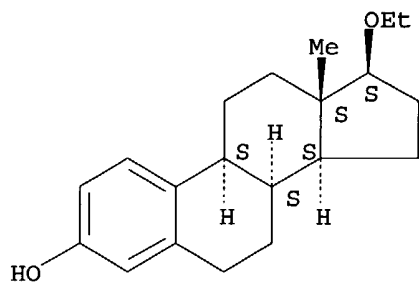
SR CA

LC STN Files: CA, CAPLUS, CASREACT

DT.CA Caplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Relative stereochemistry.



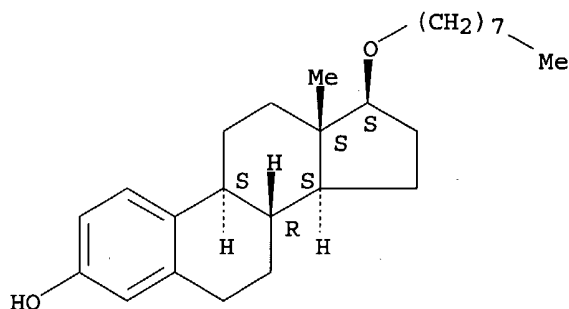
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:381661

L21 ANSWER 2 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 319427-07-1 REGISTRY  
CN Estra-1,3,5(10)-trien-3-ol, 17-(octyloxy)-, (17β)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C26 H40 O2  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL  
DT.CA Caplus document type: Journal; Patent  
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)  
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PRP (Properties)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)  
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:85991

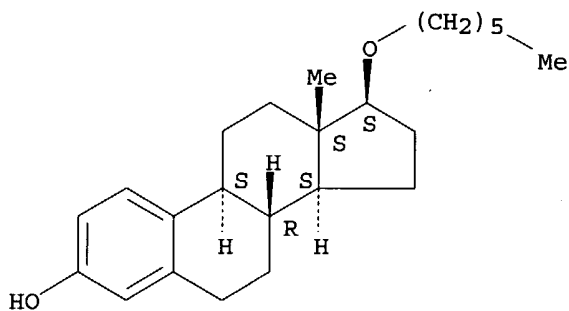
REFERENCE 2: 135:221441

REFERENCE 3: 134:101056

L21 ANSWER 3 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN

RN 319427-06-0 REGISTRY  
 CN Estra-1,3,5(10)-trien-3-ol, 17-(hexyloxy)-, (17 $\beta$ )- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C24 H36 O2  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL  
 DT.CA Caplus document type: Journal; Patent  
 RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)  
 RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

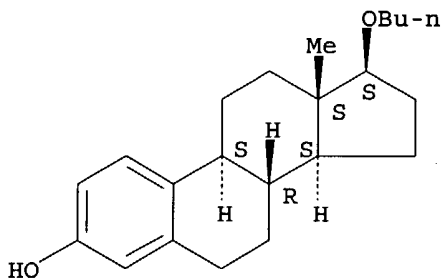
2 REFERENCES IN FILE CA (1907 TO DATE)  
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

L21 ANSWER 4 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 319427-05-9 REGISTRY  
 CN Estra-1,3,5(10)-trien-3-ol, 17-butoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C22 H32 O2  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL  
 DT.CA Caplus document type: Journal; Patent  
 RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); PRP (Properties); USES (Uses)  
 RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PRP (Properties)

Absolute stereochemistry.



## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

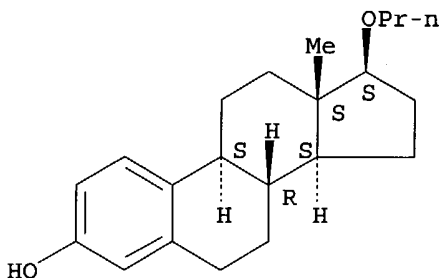
2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

L21 ANSWER 5 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 319427-04-8 REGISTRY  
CN Estra-1,3,5(10)-trien-3-ol, 17-propoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C21 H30 O2  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL  
DT.CA Caplus document type: Journal; Patent  
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)  
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PRP (Properties)

Absolute stereochemistry.



## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)  
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

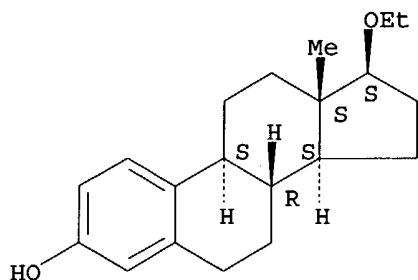
REFERENCE 1: 138:214660

REFERENCE 2: 136:85991

REFERENCE 3: 134:101056

L21 ANSWER 6 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 319427-03-7 REGISTRY  
CN Estra-1,3,5(10)-trien-3-ol, 17-ethoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C20 H28 O2  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL  
DT.CA Caplus document type: Journal; Patent  
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)  
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

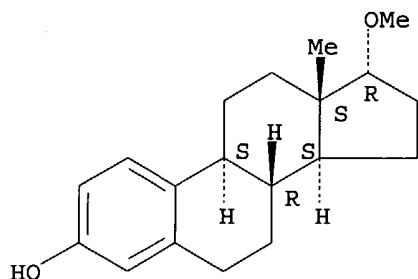
2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

L21 ANSWER 7 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 182823-27-4 REGISTRY  
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17α)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C19 H26 O2  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL  
DT.CA Caplus document type: Patent  
RL.P Roles from patents: BIOL (Biological study); USES (Uses)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

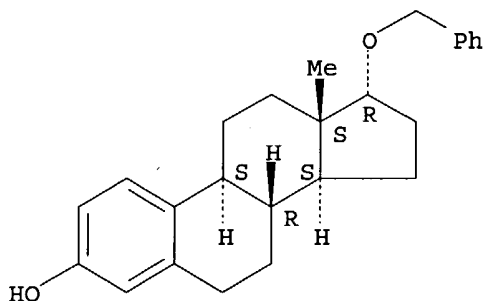
1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 125:294029

L21 ANSWER 8 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 182624-51-7 REGISTRY  
CN Estra-1,3,5(10)-trien-3-ol, 17-(phenylmethoxy)-, (17α)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C25 H30 O2

SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL  
 DT.CA Caplus document type: Patent  
 RL.P Roles from patents: BIOL (Biological study); USES (Uses)

Absolute stereochemistry.



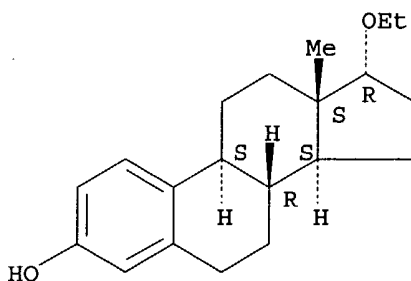
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1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 125:294029

L21 ANSWER 9 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 182624-49-3 REGISTRY  
 CN Estra-1,3,5(10)-trien-3-ol, 17-ethoxy-, (17α)- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C20 H28 O2  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL  
 DT.CA Caplus document type: Patent  
 RL.P Roles from patents: BIOL (Biological study); USES (Uses)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

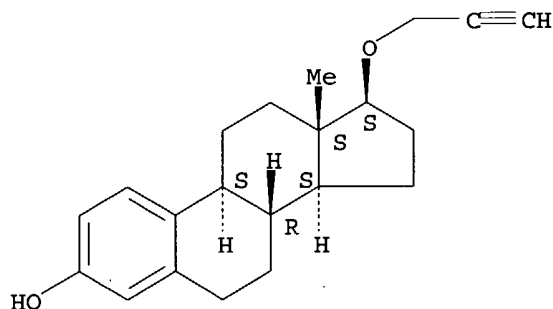
1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 125:294029

L21 ANSWER 10 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 126003-44-9 REGISTRY

CN Estra-1,3,5(10)-trien-3-ol, 17-(2-propynyloxy)-, (17 $\beta$ )- (9CI) (CA  
 INDEX NAME)  
 FS STEREOSEARCH  
 MF C21 H26 O2  
 SR CA  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
 (\*File contains numerically searchable property data)  
 DT.CA Caplus document type: Journal  
 RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 117:8261

REFERENCE 2: 112:158724

L21 ANSWER 11 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN

RN 119309-39-6 REGISTRY

CN Estra-1,3,5(10)-trien-3-ol, 17-(2-methylpropoxy)-, (17 $\alpha$ )- (9CI) (CA  
 INDEX NAME)

OTHER NAMES:

CN 17 $\alpha$ -Isobutylestradiol

FS STEREOSEARCH

MF C22 H32 O2

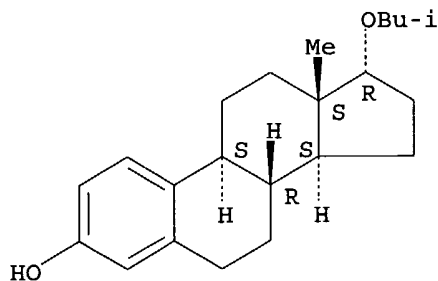
SR CA

LC STN Files: CA, CAPLUS

DT.CA Caplus document type: Journal

RL.NP Roles from non-patents: ANST (Analytical study)

Absolute stereochemistry.



**\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\***

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 113:29367

REFERENCE 2: 110:121535

L21 ANSWER 12 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN

RN 100017-39-8 REGISTRY

CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (8 $\alpha$ ,17 $\beta$ )- (9CI) (CA  
INDEX NAME)

FS STEREOSEARCH

MF C19 H26 O2

SR CA

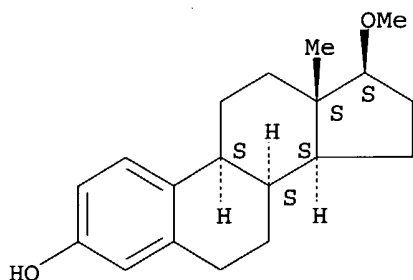
LC STN Files: BEILSTEIN\*, CA, CAPLUS

(\*File contains numerically searchable property data)

DT.CA Caplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation)

Absolute stereochemistry.

**\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\***

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 104:62244

L21 ANSWER 13 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN

RN 88247-77-2 REGISTRY

CN Estra-1,3,5(10)-trien-6,9-t2-3-ol, 17-(cyclopentyloxy)-, (17 $\beta$ )- (9CI)  
(CA INDEX NAME)

FS STEREOSEARCH

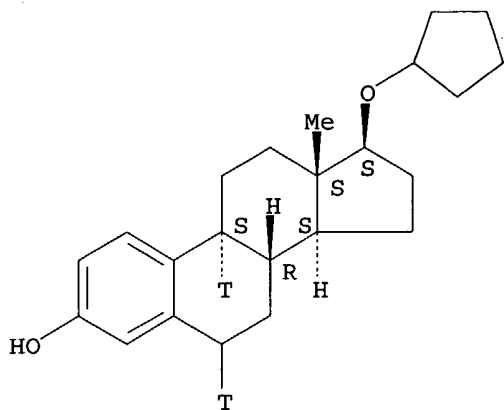
MF C23 H30 O2 T2

LC STN Files: CA, CAPLUS

DT.CA Caplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties)

Absolute stereochemistry.

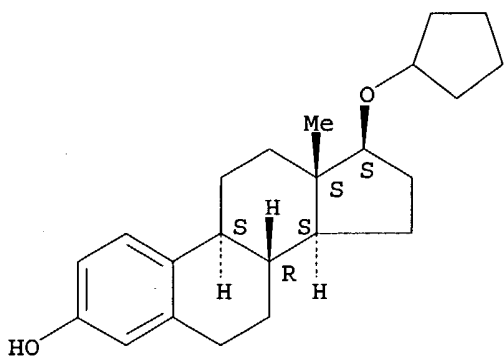


1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 100:22887

L21 ANSWER 14 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 85391-72-6 REGISTRY  
CN Estra-1,3,5(10)-trien-3-ol, 17-(cyclopentyloxy)-, (17β)- (9CI) (CA  
INDEX NAME)  
FS STEREOSEARCH  
MF C23 H32 O2  
SR European Union (EU)  
LC STN Files: CA, CAPLUS, CHEMLIST  
Other Sources: EINECS\*\*  
(\*\*Enter CHEMLIST File for up-to-date regulatory information)  
DT.CA Caplus document type: Journal  
RL.NP Roles from non-patents: RACT (Reactant or reagent)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

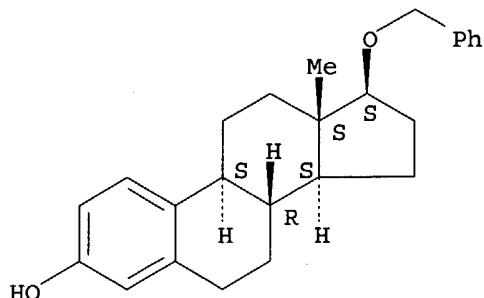
1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 100:22887

L21 ANSWER 15 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 55561-42-7 REGISTRY

CN Estra-1,3,5(10)-trien-3-ol, 17-(phenylmethoxy)-, (17 $\beta$ )- (9CI) (CA  
 INDEX NAME)  
 FS STEREOSEARCH  
 MF C25 H30 O2  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, USPATFULL  
 (\*File contains numerically searchable property data)  
 DT.CA Caplus document type: Journal; Patent  
 RL.P Roles from patents: BIOL (Biological study); USES (Uses)  
 RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.



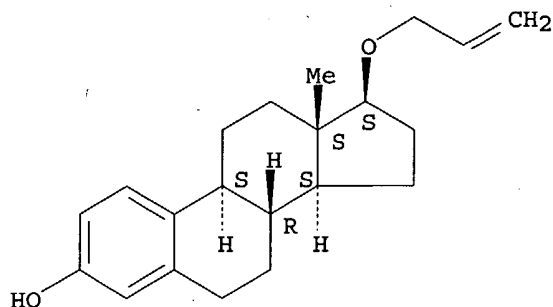
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

6 REFERENCES IN FILE CA (1907 TO DATE)  
 6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:187955  
 REFERENCE 2: 138:44718  
 REFERENCE 3: 117:170477  
 REFERENCE 4: 114:246452  
 REFERENCE 5: 90:202998  
 REFERENCE 6: 82:125520

L21 ANSWER 16 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 55561-41-6 REGISTRY  
 CN Estra-1,3,5(10)-trien-3-ol, 17-(2-propenyloxy)-, (17 $\beta$ )- (9CI) (CA  
 INDEX NAME)  
 FS STEREOSEARCH  
 MF C21 H28 O2  
 LC STN Files: CA, CAPLUS  
 DT.CA Caplus document type: Journal; Patent  
 RL.P Roles from patents: RACT (Reactant or reagent)  
 RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 86:90134

REFERENCE 2: 82:125520

L21 ANSWER 17 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN

RN 41622-69-9 REGISTRY

CN Estradiol, 17-(1-allyloxy)-, (17β)- (9CI)  
(CA INDEX NAME)

OTHER NAMES:

CN 17β-(1-allyloxy)estradiol

FS STEREOSEARCH

MF C26 H36 O2

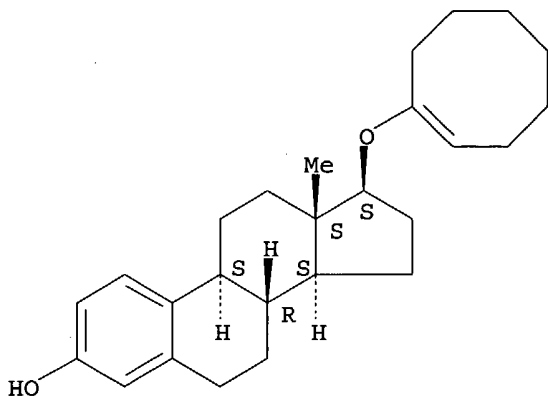
LC STN Files: CA, CAPLUS, CASREACT

DT.CA Caplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation)

Absolute stereochemistry.

Double bond geometry unknown.



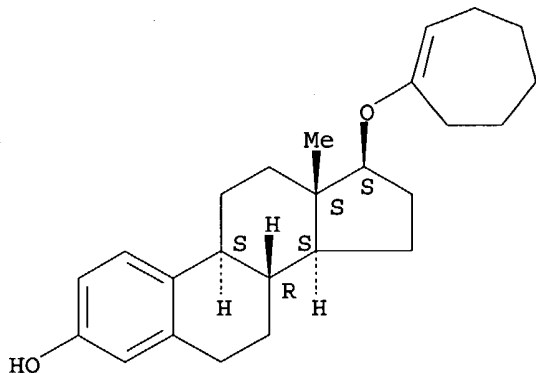
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1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 78:106316

L21 ANSWER 18 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 41622-66-6 REGISTRY  
 CN Estra-1,3,5(10)-trien-3-ol, 17-(1-cyclohepten-1-yloxy)-, (17 $\beta$ )- (9CI)  
 (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C25 H34 O2  
 LC STN Files: CA, CAPLUS  
 DT.CA Caplus document type: Journal  
 RL.NP Roles from non-patents: PREP (Preparation)

Absolute stereochemistry.



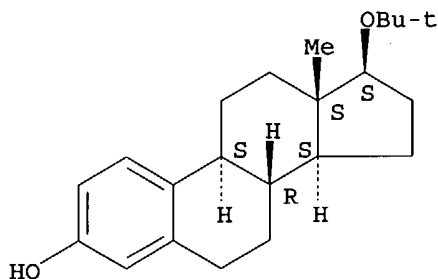
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1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 78:106316

L21 ANSWER 19 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 38781-59-8 REGISTRY  
 CN Estra-1,3,5(10)-trien-3-ol, 17-(1,1-dimethylethoxy)-, (17 $\beta$ )- (9CI)  
 (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C22 H32 O2  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS  
 (\*File contains numerically searchable property data)  
 DT.CA Caplus document type: Journal  
 RL.NP Roles from non-patents: BIOL (Biological study); RACT (Reactant or reagent)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)  
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 85:154233

REFERENCE 2: 80:121187

REFERENCE 3: 77:101990

L21 ANSWER 20 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN

RN 13885-34-2 REGISTRY

CN Estra-1,3,5(10)-trien-3-ol, 17-(1-cyclohexen-1-yloxy)-, (17 $\beta$ )- (9CI)  
(CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Estra-1,3,5(10)-trien-3-ol, 17 $\beta$ -(1-cyclohexen-1-yloxy)- (8CI)

FS STEREOSEARCH

MF C24 H32 O2

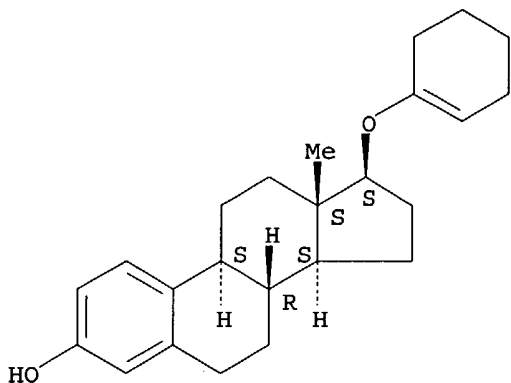
LC STN Files: BEILSTEIN\*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB  
(\*File contains numerically searchable property data)

DT.CA Caplus document type: Journal; Patent

RL.P Roles from patents: PREP (Preparation)

RL.NP Roles from non-patents: PREP (Preparation)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)  
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 78:106316

REFERENCE 2: 70:68634

REFERENCE 3: 66:95293

L21 ANSWER 21 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN

RN 13885-30-8 REGISTRY

CN Estra-1,3,5(10)-trien-3-ol, 17 $\beta$ -(1-cyclopenten-1-yloxy)- (8CI) (CA  
INDEX NAME)

FS STEREOSEARCH

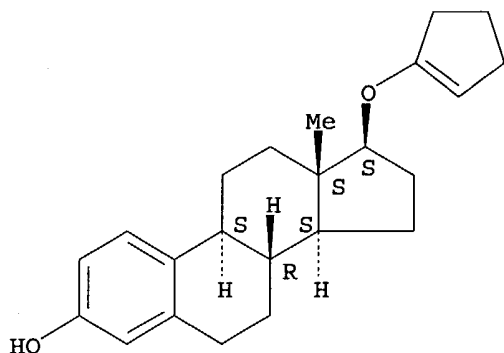
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LC STN Files: BEILSTEIN\*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB  
(\*File contains numerically searchable property data)

DT.CA Caplus document type: Patent

RL.P Roles from patents: PREP (Preparation)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 70:68634

REFERENCE 2: 66:95293

L21 ANSWER 22 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN

RN 4954-12-5 REGISTRY

CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Estra-1,3,5(10)-trien-3-ol, 17 $\beta$ -methoxy- (7CI, 8CI)

OTHER NAMES:

CN 17-Methoxy-1,3,5(10)-estratrien-3-ol

CN 17 $\beta$ -Methoxyestra-1,3,5(10)-trien-3-ol

FS STEREOSEARCH

MF C19 H26 O2

LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, CASREACT, TOXCENTER, USPATFULL  
(\*File contains numerically searchable property data)

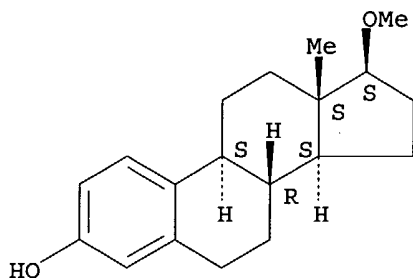
DT.CA Caplus document type: Conference; Journal; Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

RL.NP Roles from non-patents: BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); NORL (No role in record)

RLD.NP Roles for non-specific derivatives from non-patents: PREP (Preparation); PRP (Properties)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

20 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 20 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 138:348841  
 REFERENCE 2: 136:85991  
 REFERENCE 3: 134:101056  
 REFERENCE 4: 130:293190  
 REFERENCE 5: 129:54482  
 REFERENCE 6: 116:235946  
 REFERENCE 7: 100:96847  
 REFERENCE 8: 89:2201  
 REFERENCE 9: 86:90134  
 REFERENCE 10: 82:125520

=> => d his l61

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FILE 'HCAPLUS' ENTERED AT 11:29:20 ON 20 JUL 2004

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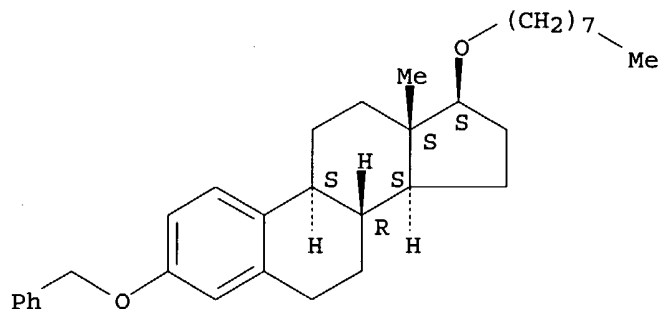
L61 10 S L5 NOT L21

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L61 ANSWER 1 OF 10 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 319427-02-6 REGISTRY  
 CN Estra-1,3,5(10)-triene, 17-(octyloxy)-3-(phenylmethoxy)-, (17 $\beta$ )-(9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C33 H46 O2  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL

DT.CA Caplus document type: Journal; Patent  
 RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)  
 RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

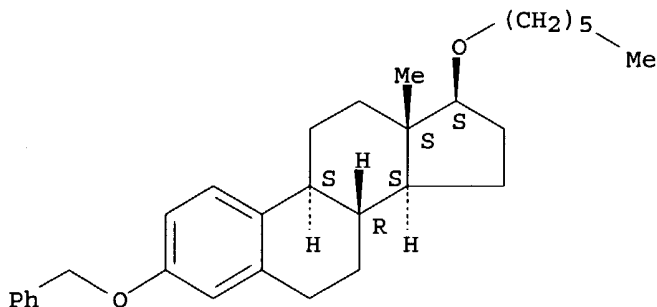
2 REFERENCES IN FILE CA (1907 TO DATE)  
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

L61 ANSWER 2 OF 10 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 319427-01-5 REGISTRY  
 CN Estra-1,3,5(10)-triene, 17-(hexyloxy)-3-(phenylmethoxy)-, (17β)-  
 (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C31 H42 O2  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL  
 DT.CA Caplus document type: Journal; Patent  
 RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)  
 RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

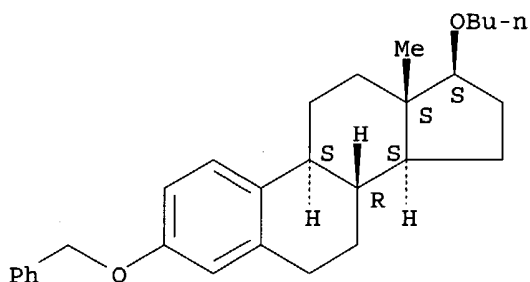
2 REFERENCES IN FILE CA (1907 TO DATE)  
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

L61 ANSWER 3 OF 10 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 319427-00-4 REGISTRY  
CN Estra-1,3,5(10)-triene, 17-butoxy-3-(phenylmethoxy)-, (17 $\beta$ )- (9CI)  
(CA INDEX NAME)  
FS STEREOSEARCH  
MF C29 H38 O2  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL  
DT.CA Caplus document type: Journal; Patent  
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)  
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

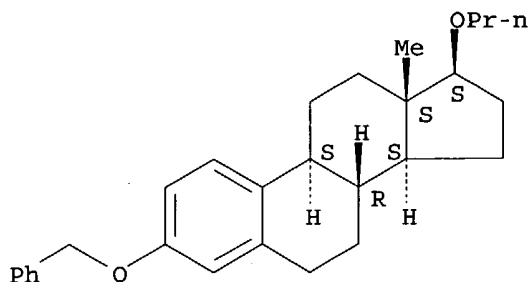
2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

L61 ANSWER 4 OF 10 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 319426-99-8 REGISTRY  
CN Estra-1,3,5(10)-triene, 3-(phenylmethoxy)-17-propoxy-, (17 $\beta$ )- (9CI)  
(CA INDEX NAME)  
FS STEREOSEARCH  
MF C28 H36 O2  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL  
DT.CA Caplus document type: Journal; Patent  
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)  
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

L61 ANSWER 5 OF 10 REGISTRY COPYRIGHT 2004 ACS on STN

RN 319426-98-7 REGISTRY

CN Estra-1,3,5(10)-triene, 17-ethoxy-3-(phenylmethoxy)-, (17β)- (9CI)  
(CA INDEX NAME)

FS STEREOSEARCH

MF C27 H34 O2

SR CA

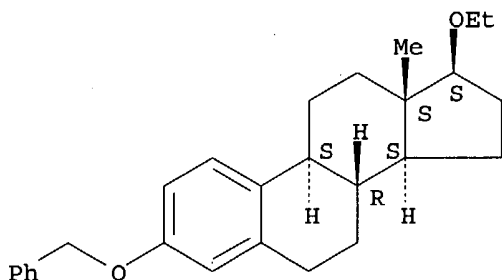
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

DT.CA Caplus document type: Journal; Patent

RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

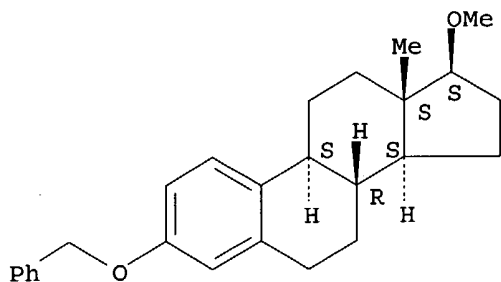
L61 ANSWER 6 OF 10 REGISTRY COPYRIGHT 2004 ACS on STN

RN 141318-37-8 REGISTRY

CN Estra-1,3,5(10)-triene, 17-methoxy-3-(phenylmethoxy)-, (17β)- (9CI)  
(CA INDEX NAME)

FS STEREOSEARCH  
 MF C26 H32 O2  
 SR CA  
 LC STN Files: CA, CAPLUS, CASREACT, USPATFULL  
 DT.CA Caplus document type: Journal; Patent  
 RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)  
 RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)  
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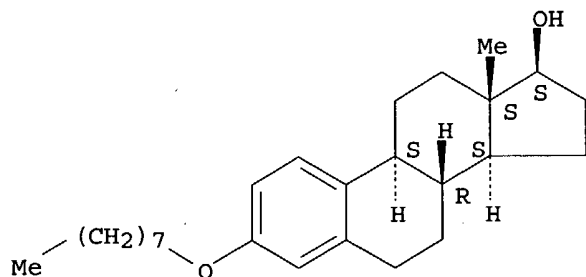
REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

REFERENCE 3: 116:235946

L61 ANSWER 7 OF 10 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 128805-68-5 REGISTRY  
 CN Estra-1,3,5(10)-trien-17-ol, 3-(octyloxy)-, (17 $\beta$ )- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C26 H40 O2  
 SR CA  
 LC STN Files: CA, CAPLUS, CASREACT, USPATFULL  
 DT.CA Caplus document type: Journal; Patent  
 RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)  
 RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)  
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

REFERENCE 3: 114:218696

L61 ANSWER 8 OF 10 REGISTRY COPYRIGHT 2004 ACS on STN

RN 21830-24-0 REGISTRY

CN Estra-1,3,5(10)-trien-17-ol, 3-butoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Estra-1,3,5(10)-trien-17 $\beta$ -ol, 3-butoxy- (8CI)

FS STEREOSEARCH

MF C22 H32 O2

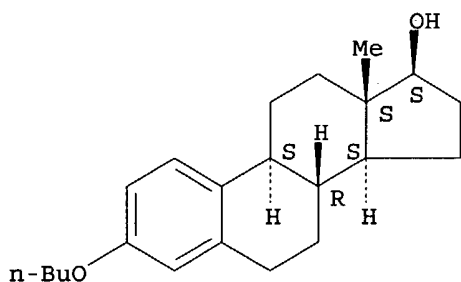
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

DT.CA Caplus document type: Journal; Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

5 REFERENCES IN FILE CA (1907 TO DATE)  
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

REFERENCE 3: 122:282544

REFERENCE 4: 71:19218

REFERENCE 5: 70:97043

L61 ANSWER 9 OF 10 REGISTRY COPYRIGHT 2004 ACS on STN

RN 14982-15-1 REGISTRY

CN Estra-1,3,5(10)-trien-17-ol, 3-(phenylmethoxy)-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Estra-1,3,5(10)-trien-17 $\beta$ -ol, 3-(benzyloxy)- (7CI, 8CI)

OTHER NAMES:

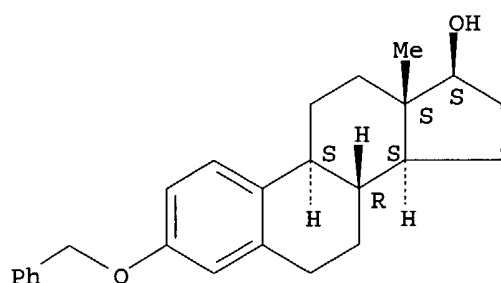
CN 3-(Benzyloxy)estra-1,3,5(10)-trien-17 $\beta$ -ol

CN 3-O-Benzylestradiol

CN BLE 99051

CN Estradiol 3-benzyl ether  
 FS STEREOSEARCH  
 MF C25 H30 O2  
 LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, CASREACT, TOXCENTER, USPATFULL  
 (\*File contains numerically searchable property data)  
 DT.CA Caplus document type: Journal; Patent  
 RL.P Roles from patents: PREP (Preparation); PROC (Process); RACT (Reactant or reagent); NORL (No role in record)  
 RL.NP Roles from non-patents: BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)

Absolute stereochemistry.



**\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\***

36 REFERENCES IN FILE CA (1907 TO DATE)  
 36 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 136:216934  
 REFERENCE 2: 136:85991  
 REFERENCE 3: 135:77015  
 REFERENCE 4: 134:326652  
 REFERENCE 5: 134:101056  
 REFERENCE 6: 131:88083  
 REFERENCE 7: 128:115126  
 REFERENCE 8: 124:270254  
 REFERENCE 9: 122:56574  
 REFERENCE 10: 120:253366

L61 ANSWER 10 OF 10 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 50-28-2 REGISTRY  
 CN Estra-1,3,5(10)-triene-3,17-diol (17 $\beta$ )- (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN Estradiol (8CI)  
 OTHER NAMES:  
 CN (+)-3,17 $\beta$ -Estradiol  
 CN  $\beta$ -Estradiol

CN 13 $\beta$ -Methyl-1,3,5(10)-gonatriene-3,17 $\beta$ -ol  
CN 17 $\beta$ -Estradiol  
CN 17 $\beta$ -Oestradiol  
CN 3,17-Epidihydroxyestratriene  
CN 3,17 $\beta$ -Dihydroxyestra-1,3,5(10)-triene  
CN 3,17 $\beta$ -Estradiol  
CN Aerodiol  
CN Altrad  
CN Aquadiol  
CN Bardiol  
CN Beta-estradiol  
CN Climaderm  
CN Climara  
CN Compudose  
CN Compudose 200  
CN Compudose 365  
CN Corpagen  
CN Dermestril  
CN Dihydrofollicular hormone  
CN Dihydrofolliculin  
CN Dihydromenformon  
CN Dihydrotheelin  
CN Dihydroxyestrin  
CN Dimenformon  
CN Diogyn  
CN Diogynets  
CN Divigel  
CN E 2  
CN Encore  
CN Epiestriol 50  
CN Estra-1,3,5(10)-triene-3,17-diol, (17 $\beta$ )-  
CN Estra-1,3,5(10)-triene-3,17 $\beta$ -diol  
CN Estrace  
CN Estraderm  
CN Estraderm TTS  
CN Estraderm TTS 100  
CN Estraderm TTS 50  
CN Estradot  
CN Estraldine  
CN Estring Vaginal Ring  
CN Estroclim  
CN Estroclim 50  
CN Estrogel  
CN Estrovite  
CN Evorel  
CN Femanest  
CN Femestral

ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT - Use FCN, FIDE, or ALL for  
DISPLAY

FS STEREOSEARCH

MF C18 H24 O2

CI COM

LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN\*,  
BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS,  
CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHM,  
CSNB, DDFU, DETHERM\*, DIOGENES, DRUGU, EMBASE, GMELIN\*, HODOC\*, HSDB\*,  
IFICDB, IFIPAT, IFIUDB, IMSCOSEARCH, IMSDRUGNEWS, IMSRESEARCH, IPA,  
MEDLINE, MRCK\*, MSDS-OHS, NAPRALERT, NIOSHTIC, PHAR, PIRA, PROMT,  
PROUSDDR, PS, RTECS\*, SPECINFO, SYNTHLINE, TOXCENTER, ULIDAT, USAN,  
USPAT2, USPATFULL, VETU

(\*File contains numerically searchable property data)

Other Sources: EINECS\*\*, WHO

(\*\*Enter CHEMLIST File for up-to-date regulatory information)

DT.CA CAplus document type: Book; Conference; Dissertation; Journal; Patent; Report

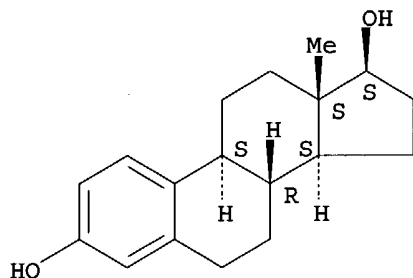
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)

RLD.P Roles for non-specific derivatives from patents: ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)

RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

52413 REFERENCES IN FILE CA (1907 TO DATE)  
 871 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 52493 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 12 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 141:53559

REFERENCE 2: 141:53482

REFERENCE 3: 141:53474

REFERENCE 4: 141:52760

REFERENCE 5: 141:52323

REFERENCE 6: 141:52267

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REFERENCE 9: 141:52046

REFERENCE 10: 141:51817

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 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
 COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

PRE-1967 CHEMICAL ABSTRACTS FILE WITH HOUR-BASED PRICING  
 FILE COVERS 1907-1966  
 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

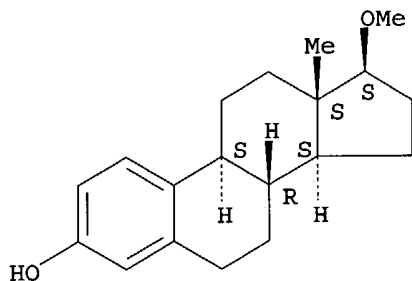
This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

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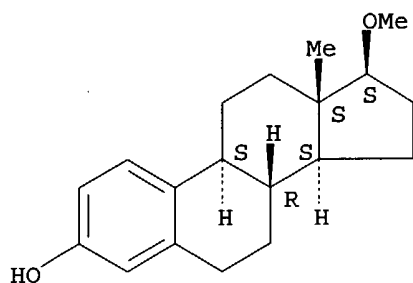
L62 ANSWER 1 OF 3 HCAOLD COPYRIGHT 2004 ACS on STN  
 AN CA64:8257g CAOLD  
 TI 17 $\beta$ -estradiol 17-methyl ether  
 AU Coombs, M. M.; Roderick, H. R.  
 TI orientation of the fragmentation in mass spectrometry by the introduction of functional groups - (VII) ethylene ketals of 2-oxosteroids  
 AU Audier, Henri; Fetizon, M.; Gramain, J. C.  
 IT 700-77-6 1743-60-8 4832-17-1 4953-96-2 **4954-12-5**  
 4954-13-6 4954-14-7 4954-16-9 4954-17-0 4967-93-5 4967-94-6  
 4967-96-8 4967-97-9 4968-11-0 4999-72-8 5380-79-0 5506-56-9  
 6857-86-9  
 IT **4954-12-5**  
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Absolute stereochemistry.



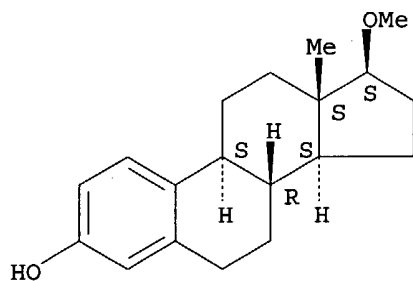
L62 ANSWER 2 OF 3 HCAOLD COPYRIGHT 2004 ACS on STN  
 AN CA61:16379g CAOLD  
 TI fractionation of estrogen methyl esters with Al2O3 column chromatography-estimation of of 16-epiestriol in pregnancy urine  
 AU Shida, Keizo; Kimura, N.; Kambegawa, A.  
 IT 1474-53-9 3434-79-5 **4954-12-5**  
 IT **4954-12-5**  
 RN 4954-12-5 HCAOLD  
 CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L62 ANSWER 3 OF 3 HCAOLD COPYRIGHT 2004 ACS on STN  
 AN CA56:7630a CAOLD  
 TI steroid derivs. - (XII) chromatography of neutral steroids on a thin Al2O3 layer  
 AU Hermanek, Stanislav; Schwarz, V.; Cekan, Z.  
 IT 113-38-2 604-32-0 633-34-1 809-51-8 1061-54-7 1169-49-9  
 1175-12-8 1182-65-6 1235-98-9 1255-57-8 1259-22-9 1639-43-6  
 1639-44-7 1807-15-4 2080-86-6 2088-71-3 2099-26-5 3604-60-2  
 4139-90-6 4651-48-3 4860-15-5 **4954-12-5** 6252-45-5  
 14072-39-0 14546-23-7 19637-35-5 20272-84-8 20867-15-6 23838-12-2  
 29163-23-3 29789-88-6 31823-53-7 33854-98-7 34209-81-9 41329-03-7  
 50303-03-2 71205-59-9 82979-88-2 95557-72-5 95908-73-9 96273-79-9  
 96275-23-9 96345-96-9 96391-62-7 96553-92-3 96772-72-4 107158-49-6  
 IT **4954-12-5**  
 RN 4954-12-5 HCAOLD  
 CN Estradiol, 17-methoxy-, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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